STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 201638

TO: Margaret Seaman
Location: rem/4C89/4C70
Art Unit: 1625
Tuesday, September 19, 2006
Case Serial Number: 10/606027

From: John DiNatale
Location: Biotech-Chem Library
REM-1B65
Phone: (571)272-2557

john.dinatale@uspto.gov

Search Notes

Examiner Seaman,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

John DiNatale
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-2557

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE CAPLUS

FILE COVERS 1907 - 19 Sep 2006 VOL 145 ISS 13
FILE LAST UPDATED: 18 Sep 2006 (20060918/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 15, 2006 (20060915/UP).

=>

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     FILE 'CAPLUS' ENTERED AT 13:41:35 ON 19 SEP 2006
L49            7 SEA ABB=ON  PLU=ON  (L45 OR L24) AND (L46 OR L47)

     FILE 'STNGUIDE' ENTERED AT 13:42:46 ON 19 SEP 2006

     FILE 'CAPLUS' ENTERED AT 13:42:53 ON 19 SEP 2006
L50           37 SEA ABB=ON  PLU=ON  TAXOL/OBI AND (L46 OR L47)

     FILE 'STNGUIDE' ENTERED AT 13:43:08 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 13:44:22 ON 19 SEP 2006

     FILE 'CAPLUS' ENTERED AT 13:44:23 ON 19 SEP 2006
               D STAT QUE L49
               D IBIB ABS HITSTR HITIND L49 1-7

     FILE 'STNGUIDE' ENTERED AT 13:46:14 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 13:47:37 ON 19 SEP 2006

     FILE 'CAPLUS' ENTERED AT 13:47:38 ON 19 SEP 2006
               D STAT QUE L24
L51           52 SEA ABB=ON  PLU=ON  L24 NOT L49
               D IBIB ABS HITSTR L51 1-52

     FILE 'STNGUIDE' ENTERED AT 13:49:23 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 13:49:31 ON 19 SEP 2006

     FILE 'CAPLUS' ENTERED AT 13:49:37 ON 19 SEP 2006
               D STAT QUE L16
               D STAT QUE L45
L52            1 SEA ABB=ON  PLU=ON  L45 AND L24
L53            0 SEA ABB=ON  PLU=ON  L45 AND L24 AND L49
               D IBIB ABS HITIND HITSTR L52 1

     FILE 'REGISTRY' ENTERED AT 13:52:04 ON 19 SEP 2006

     FILE 'CAPLUS' ENTERED AT 13:52:07 ON 19 SEP 2006
L54           13 SEA ABB=ON  PLU=ON  L45 NOT L52
               D STAT QUE L54
               D IBIB ABS HITIND HITSTR L54 1-13


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   18 SEP 2006  HIGHEST RN 907539-37-1
     DICTIONARY FILE UPDATES:  18 SEP 2006  HIGHEST RN 907539-37-1

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     Effective September 24, 2006, Concord 3D coordinates will no longer
     be available.  Please contact CAS Customer Care
     (http://www.cas.org/supp.html) if you have a need for 3D coordinates.
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L37          774 SEA ABB=ON  PLU=ON  L5 NOT L36

     FILE 'STNGUIDE' ENTERED AT 13:16:33 ON 19 SEP 2006
                D COST

     FILE 'CAPLUS' ENTERED AT 13:19:07 ON 19 SEP 2006
                E US2003-606027/APPS
L38            1 SEA ABB=ON  PLU=ON  US2003-606027/AP
                D SCA
                SEL RN

     FILE 'REGISTRY' ENTERED AT 13:19:45 ON 19 SEP 2006
L39           81 SEA ABB=ON  PLU=ON  (207680-15-7/BI OR 32981-86-5/BI OR
                352425-37-7/BI OR 352425-38-8/BI OR 352425-39-9/BI OR 352425-40
                -2/BI OR 352425-41-3/BI OR 352425-42-4/BI OR 352425-43-5/BI OR
                352425-44-6/BI OR 352425-45-7/BI OR 352425-46-8/BI OR 352425-47
                -9/BI OR 352425-48-0/BI OR 352425-49-1/BI OR 352425-50-4/BI OR
                352425-51-5/BI OR 352425-52-6/BI OR 352425-53-7/BI OR 352425-54
                -8/BI OR 352425-55-9/BI OR 352425-56-0/BI OR 352425-57-1/BI OR
                352425-58-2/BI OR 352425-59-3/BI OR 352425-60-6/BI OR 352425-61
                -7/BI OR 352425-62-8/BI OR 352425-63-9/BI OR 352425-64-0/BI OR
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                -4/BI OR 352425-69-5/BI OR 352425-70-8/BI OR 352425-72-0/BI OR
                352425-73-1/BI OR 352425-74-2/BI OR 352425-75-3/BI OR 352425-76
                -4/BI OR 352425-77-5/BI OR 352425-78-6/BI OR 352425-79-7/BI OR
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                -3/BI OR 352425-85-5/BI OR 352425-86-6/BI OR 352425-87-7/BI OR
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                -3/BI OR 352425-92-4/BI OR 352425-93-5/BI OR 352425-94-6/BI OR
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                -0/BI OR 352425-99-1/BI OR 352426-00-7/BI OR 352426-01-8/BI OR
                352426-02-9/BI OR 352426-03-0/BI OR 352426-04-1/BI OR 352426-05
                -2/BI OR 352426-06-3/BI OR 352426-07-4/BI OR 352426-08-5/BI OR
                352426-09-6/BI OR 352426-10-9/BI OR 352426-11-0/BI OR 352426-12
                -1/BI OR 352426-13-2/BI OR 352426-14-3/BI OR 352426-15-4/BI OR
                352426-16-5/BI OR 79-03-8/BI)
L40           76 SEA ABB=ON  PLU=ON  L39 AND L5
                D SCA L39

     FILE 'STNGUIDE' ENTERED AT 13:20:46 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 13:29:57 ON 19 SEP 2006
L41         4550 SEA ABB=ON  PLU=ON  11S AND L5
L42         6914 SEA ABB=ON  PLU=ON  L41 OR L8
L43          751 SEA ABB=ON  PLU=ON  L5 NOT L42
L44           51 SEA ABB=ON  PLU=ON  11R AND L5
                D SCA

     FILE 'CAPLUS' ENTERED AT 13:37:34 ON 19 SEP 2006
L45           14 SEA ABB=ON  PLU=ON  L44

     FILE 'STNGUIDE' ENTERED AT 13:38:18 ON 19 SEP 2006

     FILE 'CAPLUS' ENTERED AT 13:38:45 ON 19 SEP 2006
                E HOLTON R/AU
L46            3 SEA ABB=ON  PLU=ON  HOLTON R A/AU
L47           99 SEA ABB=ON  PLU=ON  HOLTON ROBER?/AU

     FILE 'REGISTRY' ENTERED AT 13:40:15 ON 19 SEP 2006
L48            0 SEA ABB=ON  PLU=ON  L44 AND  L22
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     FILE 'REGISTRY' ENTERED AT 11:34:17 ON 19 SEP 2006
L10             STRUCTURE UPLOADED
L11          50 SEA SUB=L5 SSS SAM L10

     FILE 'STNGUIDE' ENTERED AT 11:35:34 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 11:36:34 ON 19 SEP 2006
L12             STRUCTURE UPLOADED
L13          50 SEA SUB=L5 SSS SAM L12
               D STAT QUE L11
L14             STRUCTURE UPLOADED
L15           0 SEA SUB=L5 SSS SAM L14
L16           0 SEA SUB=L5 SSS FUL L14
               SAVE TEMP L16 SEA027STR14L/A
L17             STRUCTURE UPLOADED
L18           8 SEA SUB=L5 SSS SAM L17
               D SCA
               D STAT QUE L18
L19         203 SEA SUB=L5 SSS FUL L17

     FILE 'STNGUIDE' ENTERED AT 11:56:26 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 12:03:22 ON 19 SEP 2006
               SAVE TEMP L19 SEA027STR17L/A
L20             STRUCTURE UPLOADED
L21           6 SEA SUB=L5 SSS SAM L20
               D SCA
L22         111 SEA SUB=L5 SSS FUL L20
               SAVE TEMP L22 SEA027STR22L/A
L23          92 SEA ABB=ON  PLU=ON  L19 NOT L22

     FILE 'CAPLUS' ENTERED AT 12:18:04 ON 19 SEP 2006
L24          59 SEA ABB=ON  PLU=ON  L22

     FILE 'REGISTRY' ENTERED AT 12:22:19 ON 19 SEP 2006

     FILE 'STNGUIDE' ENTERED AT 12:27:28 ON 19 SEP 2006
               D COST

     FILE 'STNGUIDE' ENTERED AT 12:27:34 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 12:35:26 ON 19 SEP 2006
L25         101 SEA ABB=ON  PLU=ON  L22 AND L9
L26          10 SEA ABB=ON  PLU=ON  L22 NOT L25
L27         808 SEA ABB=ON  PLU=ON  L9 NOT L19
L28           6 SEA ABB=ON  PLU=ON  L27 AND STEREO
               D SCA
L29           6 SEA ABB=ON  PLU=ON  L9 AND STEREO

     FILE 'STNGUIDE' ENTERED AT 12:42:49 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 12:56:57 ON 19 SEP 2006
L30             STRUCTURE UPLOADED
L31          50 SEA SUB=L5 SSS SAM L30
L32        6747 SEA SUB=L5 SSS FUL L30
L33           2 SEA ABB=ON  PLU=ON  L8 NOT L32
               D SCA
L34             STRUCTURE UPLOADED
L35          50 SEA SUB=L5 SSS SAM L34
L36        6891 SEA SUB=L5 SSS FUL L34
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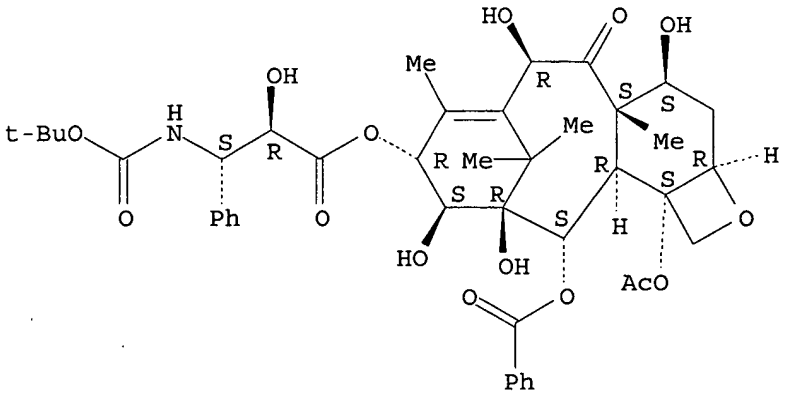

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=> d his full

     (FILE 'HOME' ENTERED AT 10:32:18 ON 19 SEP 2006)

     FILE 'REGISTRY' ENTERED AT 10:32:31 ON 19 SEP 2006
L1             1 SEA ABB=ON  PLU=ON  TAXOL/CN
                 D SCA

     FILE 'CAPLUS' ENTERED AT 10:36:03 ON 19 SEP 2006
L2         12010 SEA ABB=ON  PLU=ON  L1

     FILE 'STNGUIDE' ENTERED AT 10:36:09 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 10:58:37 ON 19 SEP 2006

     FILE 'STNGUIDE' ENTERED AT 10:59:05 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 11:00:24 ON 19 SEP 2006
L3                 STRUCTURE UPLOADED
L4              50 SEA SSS SAM L3

     FILE 'STNGUIDE' ENTERED AT 11:03:20 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 11:06:47 ON 19 SEP 2006
                   D SCA L1
                   D STAT QUE L4
L5           7665 SEA SSS FUL L3
                   SAVE TEMP SEA208STR3L/A L5
                   SAVE TEMP SEA027STR3L/A L5

     FILE 'STNGUIDE' ENTERED AT 11:10:50 ON 19 SEP 2006

     FILE 'REGISTRY' ENTERED AT 11:15:10 ON 19 SEP 2006
L6                 STRUCTURE UPLOADED
L7              50 SEA SUB=L5 SSS SAM L6
L8            6749 SEA SUB=L5 SSS FUL L6
                   SAVE TEMP SEA027STR6L/A L8
L9             916 SEA ABB=ON  PLU=ON  L5 NOT L8

     FILE 'STNGUIDE' ENTERED AT 11:29:32 ON 19 SEP 2006
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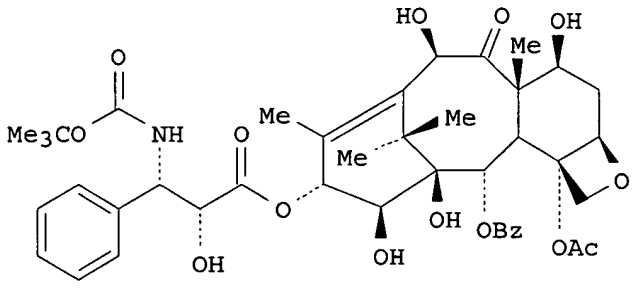
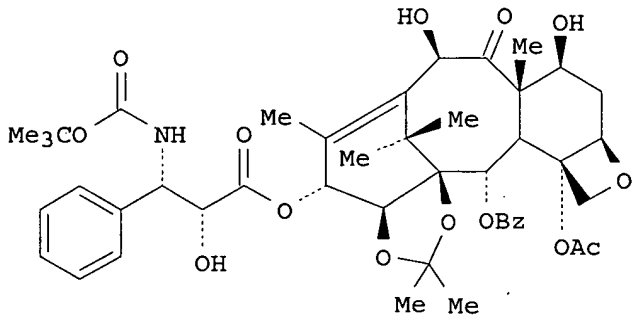


I



II

AB New taxoids, 14β-hydroxydocetaxel (I) and its 1,14-acetonide II, are synthesized from 14β-hydroxy-10-deacetylbaccatin III in good yields. The cytotoxicity of the new taxoids are evaluated against different human tumor cell lines and their ability to inhibit microtubule disassembly examined 14β-Hydroxydocetaxel shows very strong cytotoxicity, especially against A549 human non-small cell lung cancer cell line (IC50 = 0.8 nM).

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

IT 159143-49-4P **159143-50-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytotoxicity of, neoplasm inhibition in relation to)

IT **159143-50-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytotoxicity of, neoplasm inhibition in relation to)

RN 159143-50-7 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

e.g. I (R = Ph, Me3CO), were synthesized and evaluated as antitumor agents.

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

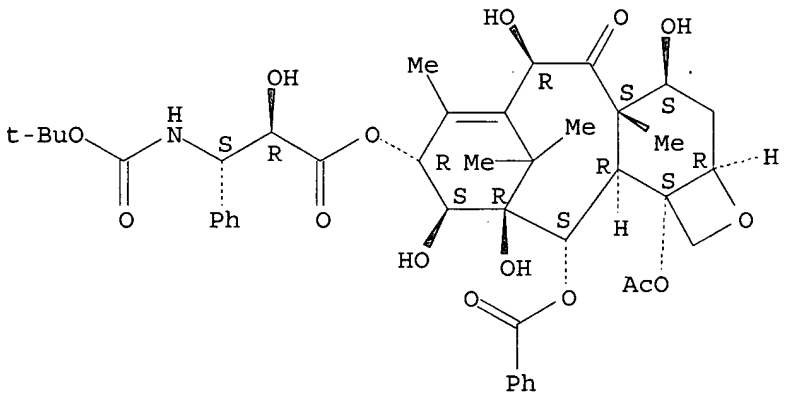
IT **159143-50-7P**, 14β-Hydroxytaxotere 159490-67-2P, 14β-Hydroxytaxol 159490-73-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and neoplasm-inhibiting activity of)

IT **159143-50-7P**, 14β-Hydroxytaxotere
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and neoplasm-inhibiting activity of)

RN 159143-50-7 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L54 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:701098 CAPLUS

DOCUMENT NUMBER: 121:301098

TITLE: Synthesis and biological activity of 14-hydroxydocetaxel

AUTHOR(S): Ojima, Iwao; Fenoglio, Ivana; Park, Young Hoon; Pera, Paula; Bernacki, Ralph J.

CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794-3400, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(13), 1571-6
CODEN: BMCLE8; ISSN: 0960-894X

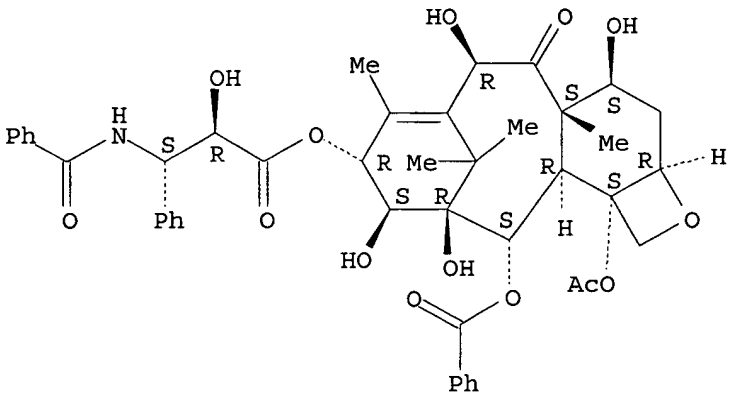
DOCUMENT TYPE: Journal

LANGUAGE: English

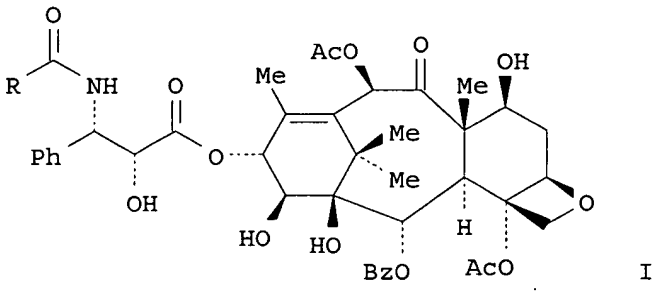
GI

RN 185623-21-6 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

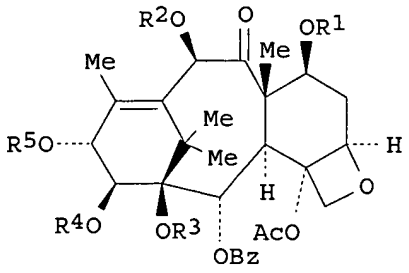


L54 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:30662 CAPLUS
DOCUMENT NUMBER: 122:10287
TITLE: Synthesis and antitumor properties of novel 14-β-hydroxytaxol and related analogs
AUTHOR(S): Kant, Joydeep; Farina, Vittorio; Fairchild, Craig; Kadow, John F.; Langley, David R.; Long, Byron H.; Rose, William C.; Vyas, Dolatrai M.
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Res. Inst., Wallingford, CT, 06492-7600, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(13), 1565-70
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:10287
GI



I

AB Novel analogs of TAXOL with an addnl. hydroxyl group at the C-14 position,



I

AB Taxane derivs. I (R1, R2, R3, R4 = independently H, alkyl, alkanoyl; R1R2, R3R4 = independently cyclic diol protecting group; R5 = H, alkyl, Ph, silyl, alkanoyl, aminoalkanoyl) were prepared from 14-β-hydroxy-10-deacetylbaccatin III (II) for use as anticancer agents. Thus, I [R1R2 = CMe2, R3 = R4 = H, R5 = (2R,3S)-PhCH(PhCONH)CH(OH)CO] was prepared via a series of synthetic steps form II and (S,S)-PhCH(NHCOPh)CH(OH)CH:CH2 and showed a 50% growth inhibition when tested against lukemia cell lines at a concns. < 0.1 μm.

IC ICM C07D305-14
ICS C07D493-18; C07D493-08; C07D413-12; A61K031-335

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

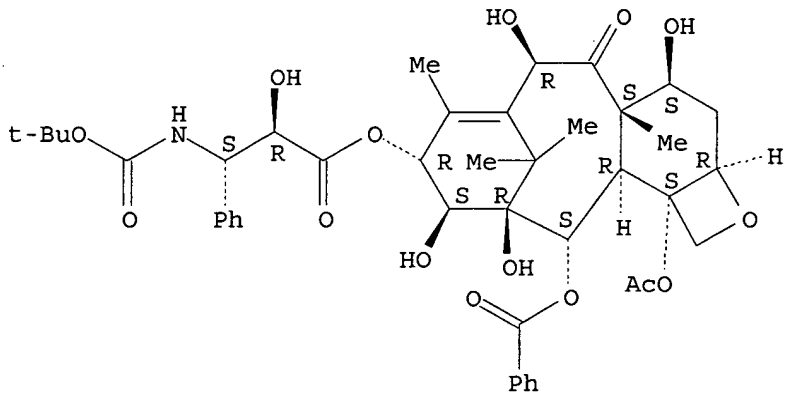
IT **159143-50-7P** 185623-14-7P 185623-15-8P 185623-16-9P
185623-21-6P 185623-28-3P 185623-35-2P 185623-39-6P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(taxane derivs. from 14-beta-hydroxy-10 deacetylbaccatin iii)

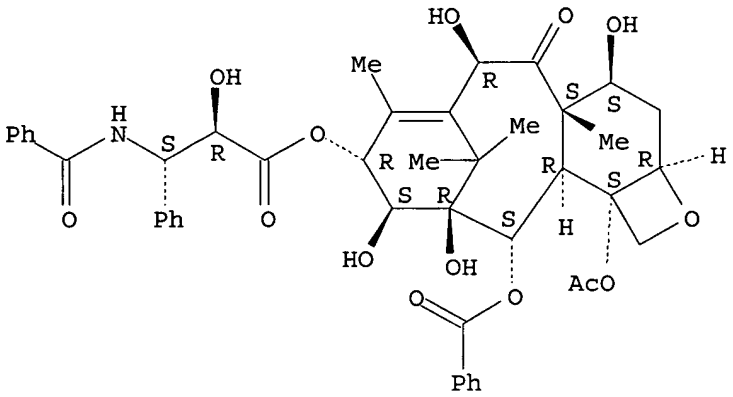
IT **159143-50-7P 185623-21-6P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(taxane derivs. from 14-beta-hydroxy-10 deacetylbaccatin iii)

RN 159143-50-7 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:77004 CAPLUS
DOCUMENT NUMBER: 126:89601
TITLE: Preparation of taxane derivatives from 14-beta-hydroxy-10-deacetylbaccatin III
INVENTOR(S): Duvvuri, Subrahmanyam; Akella, Ventakateswarlu; Vedula, Sharma Manohar; Puranik, Ramachandra; Sattegeri, Raghavendra Madhva
PATENT ASSIGNEE(S): Dr. Reddy's Research Foundation, India
SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 747372	A1	19961211	EP 1996-304031	19960604
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IT, LI, LU, NL, PT, SE				
US 5763477	A	19980609	US 1995-471639	19950606
EP 1099696	A2	20010516	EP 2001-101809	19960604
EP 1099696	A3	20010523		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, FI				

PRIORITY APPLN. INFO.:	US 1995-471639	A	19950606
	IN 1994-681	A	19940722
	IN 1994-682	A	19940722
	IN 1994-683	A	19940722
	IN 1994-684	A	19940722
	IN 1994-685	A	19940722
	EP 1996-304031	A3	19960604

OTHER SOURCE(S): MARPAT 126:89601
GI

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1, 63

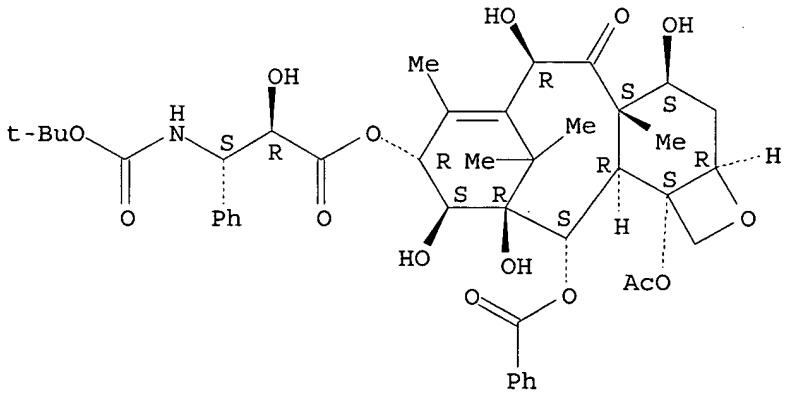
IT 156940-43-1P 156940-44-2P **159143-50-7P 185623-21-6P**
186348-05-0P, SB-T 101141 186348-07-2P 186348-08-3P, SB-T 10114
186348-09-4P, SB-T 101142 186348-10-7P, SB-T 101143 186348-11-8P, SB-T
101144 186348-13-0P, SB-T 101146 186348-15-2P, SB-T 101151
186348-23-2P, SB-T 101131 186348-24-3P, SB-T 101133 186348-25-4P, SB-T
101134
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and pharmaceutical compns. of taxanes for use as antitumor agents)

IT **159143-50-7P 185623-21-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and pharmaceutical compns. of taxanes for use as antitumor agents)

RN 159143-50-7 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 185623-21-6 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

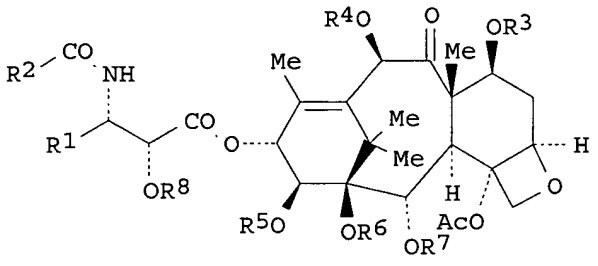
Absolute stereochemistry. Rotation (-).

CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

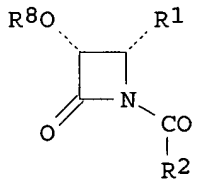
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5705508	A	19980106	US 1995-542537	19951013
US 5475011	A	19951212	US 1993-40189	19930326
CA 2158147	AA	19941013	CA 1994-2158147	19940324
CA 2158147	C	19991005		
CN 1123547	A	19960529	CN 1994-192117	19940324
CN 1067682	B	20010627		
HU 73848	A2	19960930	HU 1995-2642	19940324
CZ 288924	B6	20010912	CZ 1995-2480	19940324
PT 690856	T	20030430	PT 1994-912300	19940324
ES 2190440	T3	20030801	ES 1994-912300	19940324
US 5599820	A	19970204	US 1995-461730	19950605
JP 11322737	A2	19991124	JP 1999-102935	19990409
JP 3145993	B2	20010312		

PRIORITY APPLN. INFO.: US 1993-40189 A2 19930326
JP 1994-522192 A3 19940324

OTHER SOURCE(S): MARPAT 128:128162
GI



I



II

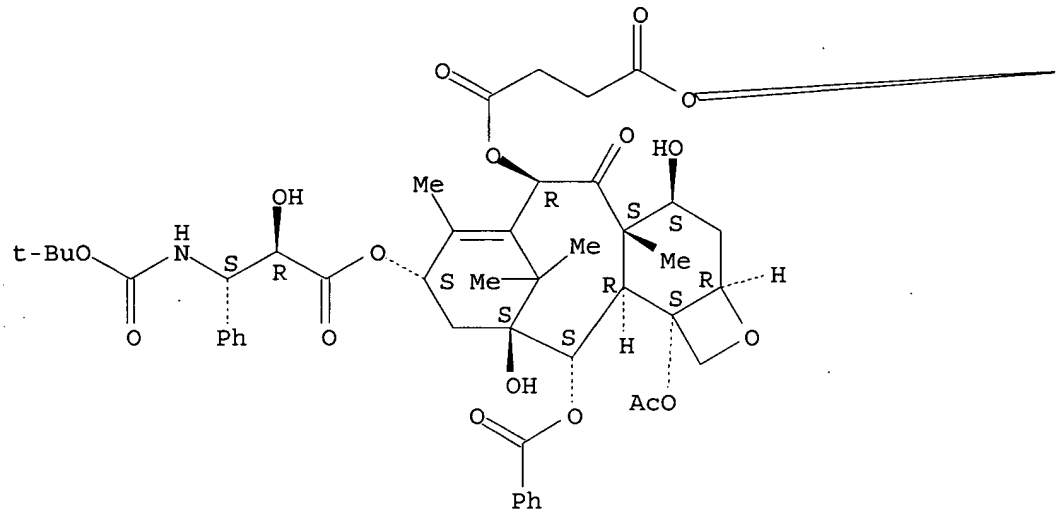
AB Taxanes I [R1 = alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl; R2 = alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, RO, RS, RR'N; R = R' = alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, R' = H; NRR' = nitrogen containing heterocyclyl; R3 = H, acyl, alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclyl; R4 = H, acyl, carbamoyl, alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclyl; R5 = R6 = H, acyl, alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclyl; R5R6 = cyclic group such as carbonate; R7 = acyl; R8 = H, hydroxy protecting group], useful as anticancer chemotherapeutic agents, were prepared via the preparation of β-lactams II and their subsequent reaction with baccatin III analogs. Thus, I [R1 = R2 = Ph, R3 = R4 = R5 = R6 = R8 = H, R7 = COPh] was prepared via O-acylation of 7O,10O-bis(2,2,2-trichloroethyloxycarbonyl)-14-hydroxy-10-deacetylbaccatin III with II [R1 = R2 = Ph, R8 = CHMeOEt]. Prepared taxanes were tested for anticancer activity against a variety of cell lines including A121 ovarian tumor cells and HT-29 colon cancer cells.

IC ICM A61K031-445
ICS C07D305-00
INCL 514320000

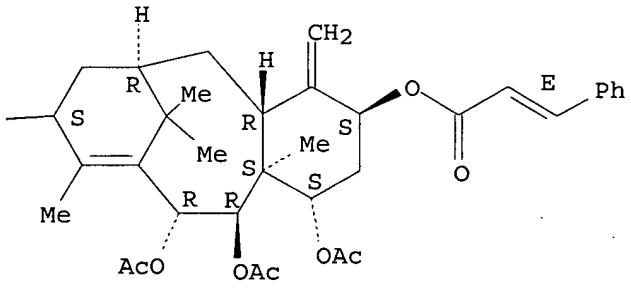
cyclodeca[3,4]benz[1,2-b]oxet-6-yl (1S,3S,4aR,6R,8S,11R,12R,12aS)-1,11,12-tris(acetyloxy)-1,2,3,4,4a,5,6,7,8,11,12,12a-dodecahydro-9,12a,13,13-tetramethyl-4-methylene-3-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-6,10-methanobenzocyclodecen-8-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:41718 CAPLUS
DOCUMENT NUMBER: 128:128162
TITLE: Preparation and pharmaceutical compositions of taxanes for use as antitumor agents
INVENTOR(S): Ojima, Iwao; Bombardelli, Ezio
PATENT ASSIGNEE(S): Research Foundation of State University of New York, USA; Indena S.p.A. of Viale Ortles
SOURCE: U.S., 27 pp., Cont.-in-part of U.S. 5,475,011.

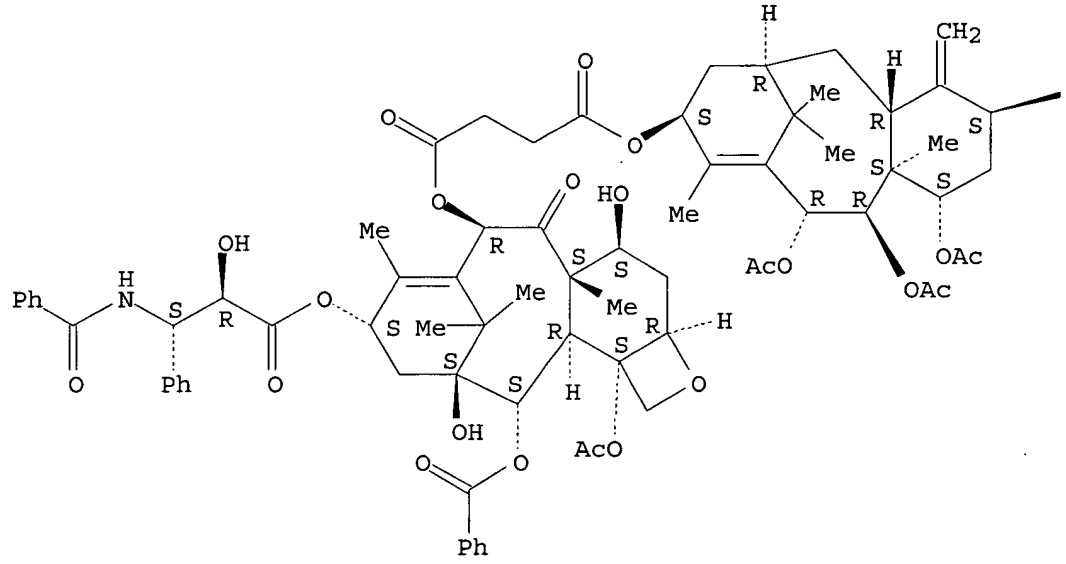
IT **237428-97-6P 237429-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and antitumor activity of paclitaxel(docetaxel)/2-deacetoxytaxinine J dimers)

RN 237428-97-6 CAPLUS

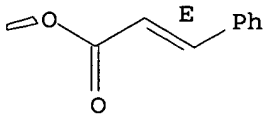
CN Butanedioic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-9-[(2R,3S)-3-(benzoylamino)-2-hydroxy-1-oxo-3-phenylpropoxy]-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl (1S,3S,4aR,6R,8S,11R,12R,12aS)-1,11,12-tris(acetyloxy)-1,2,3,4,4a,5,6,7,8,11,12,12a-dodecahydro-9,12a,13,13-tetramethyl-4-methylene-3-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-6,10-methanobenzocyclodecen-8-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

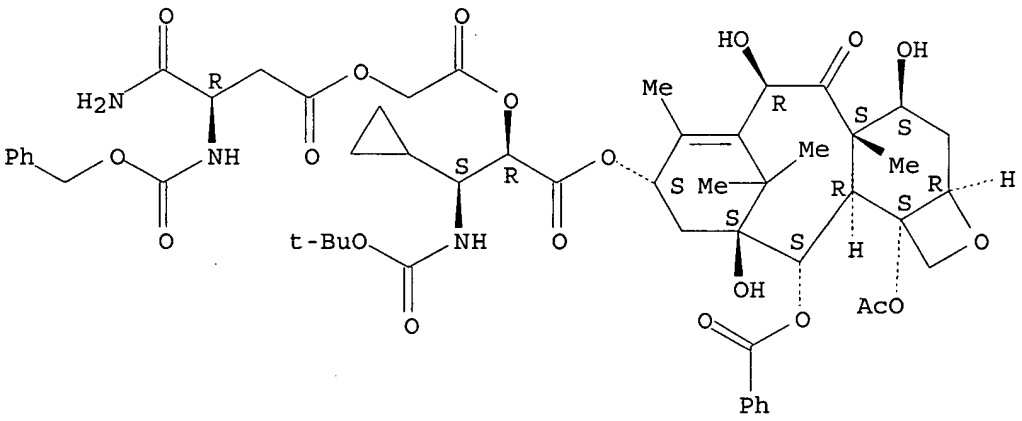


RN 237429-07-1 CAPLUS

CN Butanedioic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-9-[(2R,3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-1-oxo-3-phenylpropoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-

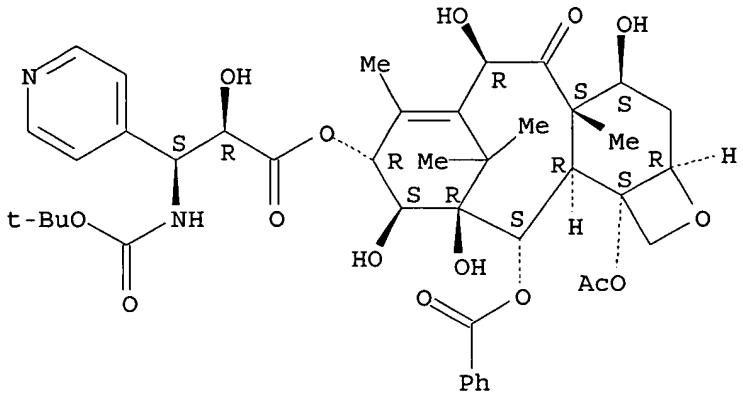
3'-desphenyl-3'-cyclopropyldocetaxel)
RN 244121-78-6 CAPLUS
CN 5,8-Dioxa-2,12-diazatridecanedioic acid, 4-[[[(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl]oxy]carbonyl]-11-(aminocarbonyl)-3-cyclopropyl-6,9-dioxo-, 1-(1,1-dimethylethyl) 13-(phenylmethyl) ester, (3S,4R,11R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:348792 CAPLUS
DOCUMENT NUMBER: 131:157845
TITLE: Chemistry and occurrence of taxane derivatives. XXXII. synthesis of paclitaxel (docetaxel)/2-deacetoxytaxinine J dimers
AUTHOR(S): Appendino, Giovanni; Belloro, Emanuela; Jakupovic, Sven; Danieli, Bruno; Jakupovic, Jasmin; Bombardelli, Ezio
CORPORATE SOURCE: Dipartimento di Scienza e Tecnologia del Farmaco, Turin, 10125, Italy
SOURCE: Tetrahedron (1999), 55(21), 6567-6576
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Starting from taxanes available in multigram amts. from widespread ornamental yews (10-deacetylbaccatin III and 2'-deacetoxyaustrospicatine), two dimeric taxoids with potential dual target specificity (β-tubulin and P-gp) were synthesized. Both compds. lacked significant cytotoxicity, though one retained a strong activity in the tubulin depolymn. assay.
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1
IT **237428-97-6P 237429-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and antitumor activity of paclitaxel(docetaxel)/2-deacetoxytaxinine J dimers)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

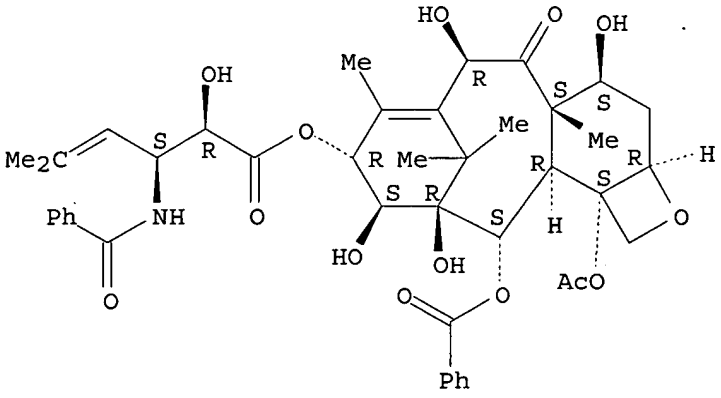
L54 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:404096 CAPLUS
DOCUMENT NUMBER: 131:243428
TITLE: Synthesis of taxoids 5. Synthesis and evaluation of novel water-soluble prodrugs of a 3'-desphenyl-3'-cyclopropyl analogue of docetaxel
AUTHOR(S): Yamaguchi, Tetsuo; Harada, Naoyuki; Ozaki, Kunihiko; Arakawa, Hiroaki; Oda, Kouji; Nakanishi, Noriyuki; Tsujihara, Kenji; Hashiyama, Tomiki
CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Tanabe Seiyaku Co., Ltd., Toda, 335-8505, Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(12), 1639-1644
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel 3'-desphenyl-3'-cyclopropyl analog of docetaxel was synthesized from 10-deacetyl-baccatin III. The cytotoxicity of the new taxoid was evaluated against several human tumor cell lines, and it had ca. 20 times stronger activity against human colon cancer cell lines (WiDr and Colon 320) than that of docetaxel. This taxoid was converted to its water-soluble prodrugs that have 2'-substituted amino acid derivs. with spacer. The prodrugs had good solubility in saline and showed more potent antitumor activity against B 16 melanoma in mice than that of docetaxel.

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

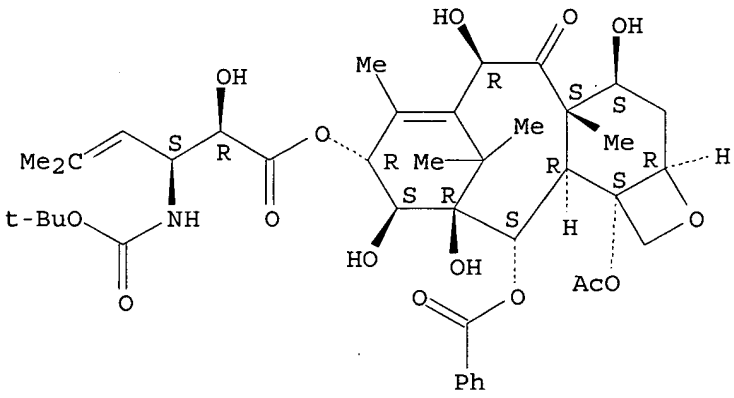
IT 178247-80-8P 178247-81-9P 178247-82-0P 178247-83-1P 178247-84-2P
178247-85-3P 178247-87-5P 178247-97-7P 178248-33-4P 178248-34-5P
178248-35-6P 178248-38-9P 205640-20-6P **244121-78-6P**
244121-79-7P 244121-80-0P 244121-81-1P 244121-82-2P 244121-83-3P
244121-84-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and antitumor activity of water-soluble prodrugs of 3'-desphenyl-3'-cyclopropyldocetaxel)

IT **244121-78-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and antitumor activity of water-soluble prodrugs of



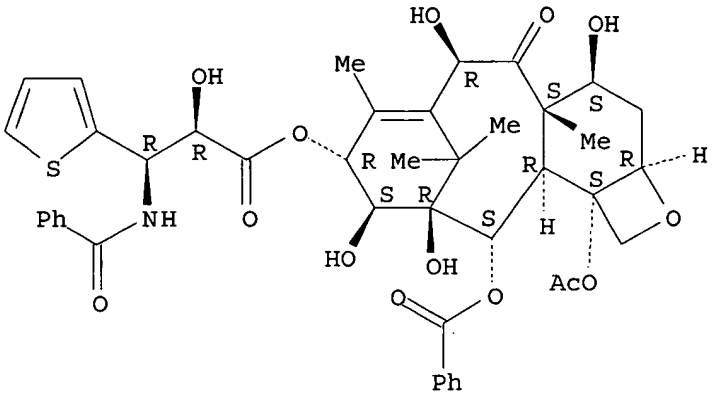
RN 232948-86-6 CAPLUS
CN 4-Hexenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



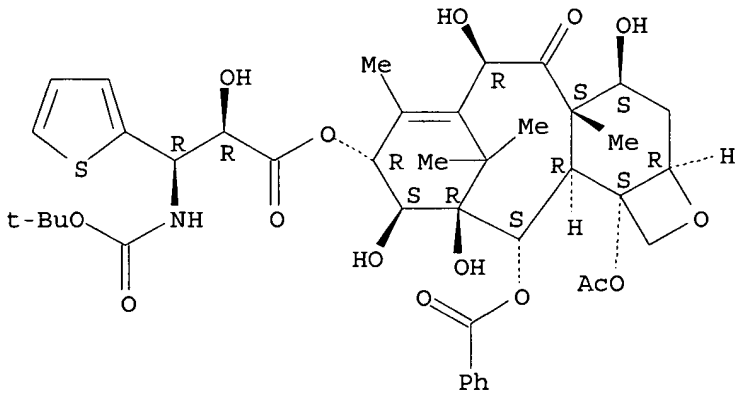
RN 232948-87-7 CAPLUS
CN 4-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



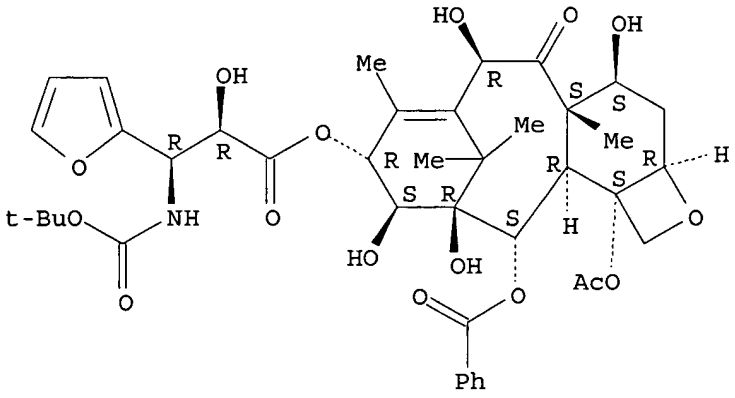
RN 232948-84-4 CAPLUS
CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



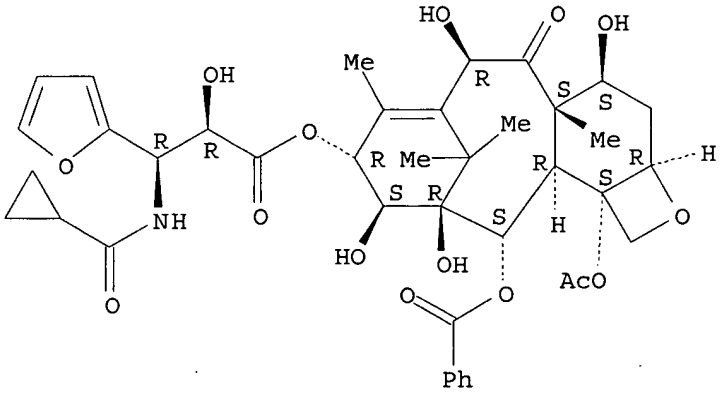
RN 232948-85-5 CAPLUS
CN 4-Hexenoic acid, 3-(benzoylamino)-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



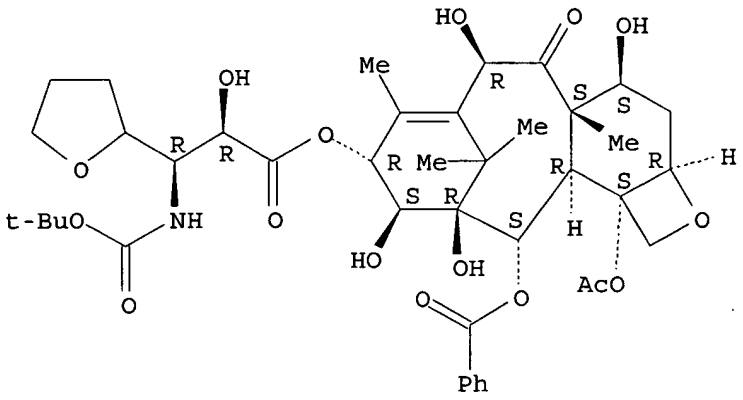
RN 232948-82-2 CAPLUS
CN 2-Furanpropanoic acid,.β-[(cyclopropylcarbonyl)amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



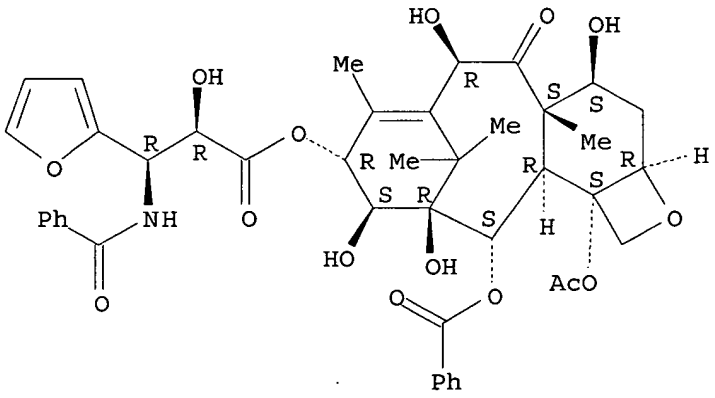
RN 232948-83-3 CAPLUS
CN 2-Thiophenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



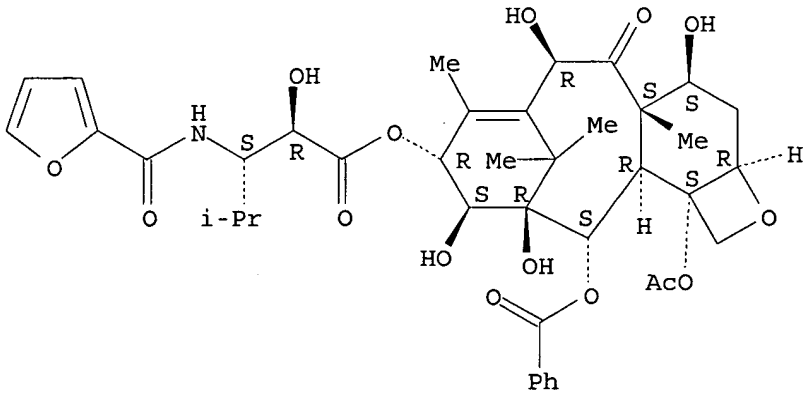
RN 232948-80-0 CAPLUS
CN 2-Furanpropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



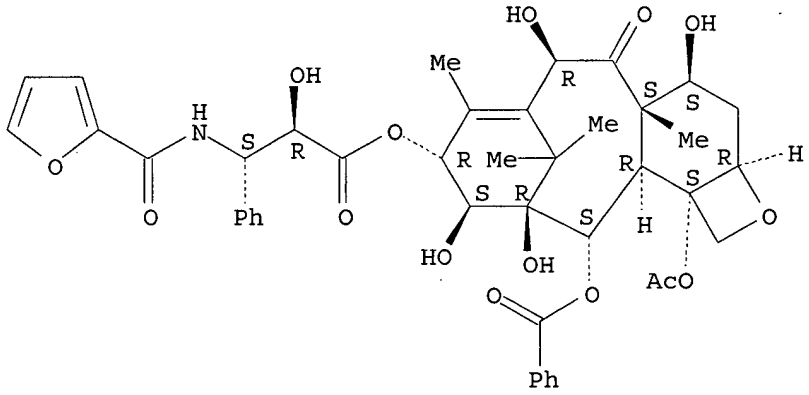
RN 232948-81-1 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



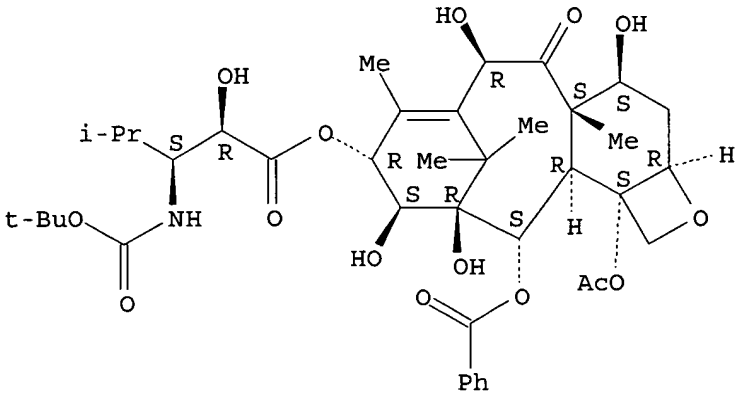
RN 232948-78-6 CAPLUS
CN Benzenepropanoic acid, β-[(2-furanylcarbonyl)amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



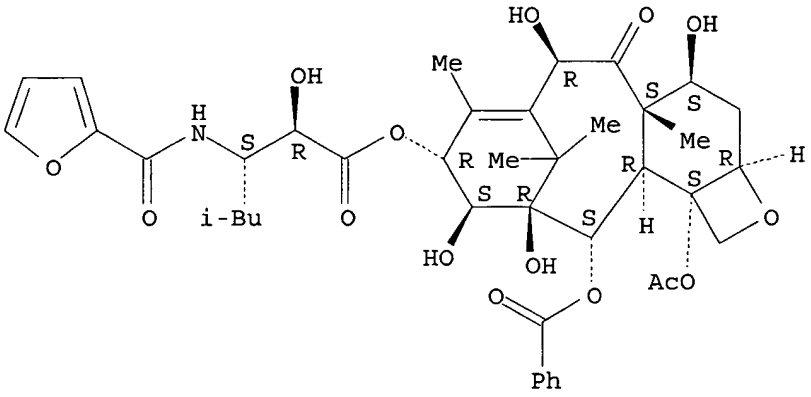
RN 232948-79-7 CAPLUS
CN L-threo-Heptonic acid, 4,7-anhydro-3,5,6-trideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



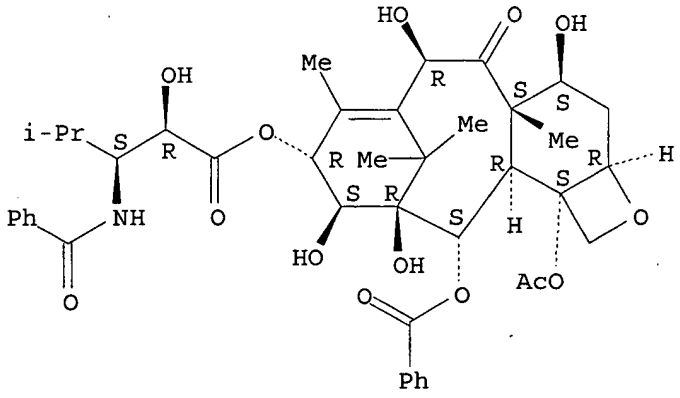
RN 232948-76-4 CAPLUS
CN Hexanoic acid, 3-[(2-furanylcarbonyl)amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



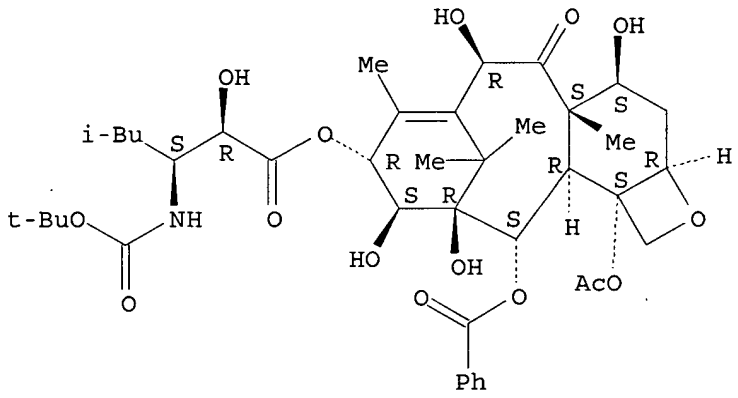
RN 232948-77-5 CAPLUS
CN L-threo-Pentonic acid, 3,4,5-trideoxy-3-[(2-furanylcarbonyl)amino]-4-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



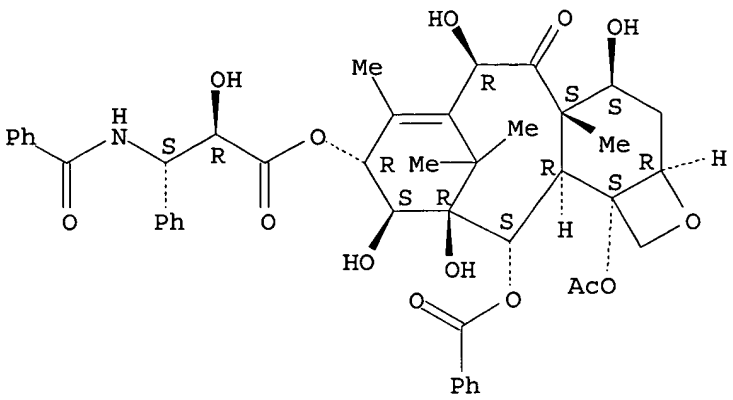
RN 232948-74-2 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



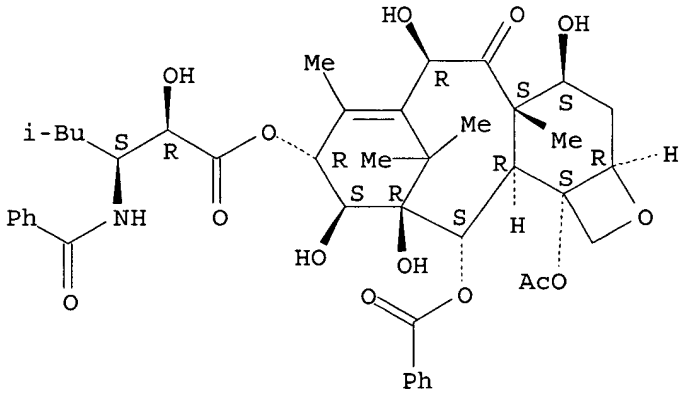
RN 232948-75-3 CAPLUS
CN L-threo-Pentonic acid, 3,4,5-trideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



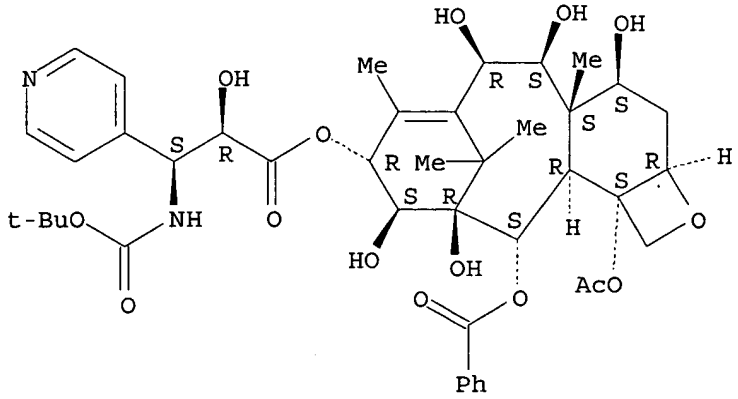
RN 232948-71-9 CAPLUS
CN Hexanoic acid, 3-(benzoylamino)-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 232948-72-0 CAPLUS
CN L-threo-Pentonic acid, 3-(benzoylamino)-3,4,5-trideoxy-4-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

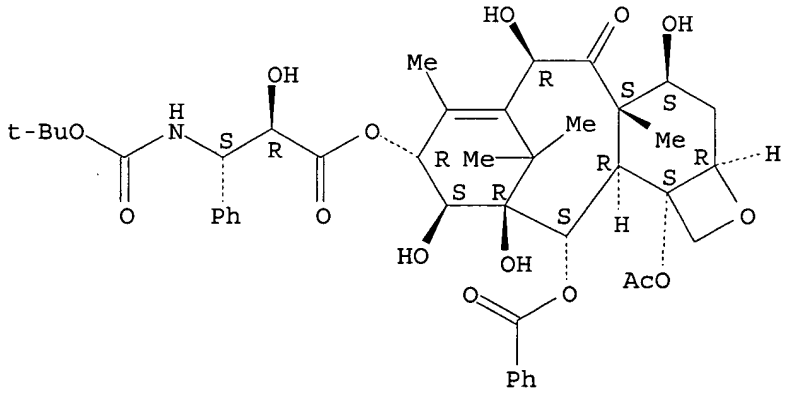


IT **159143-50-7 185623-21-6 232948-71-9**
232948-72-0 232948-74-2 232948-75-3
232948-76-4 232948-77-5 232948-78-6
232948-79-7 232948-80-0 232948-81-1
232948-82-2 232948-83-3 232948-84-4
232948-85-5 232948-86-6 232948-87-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel water soluble taxane diterpenes as anticancer agents)

RN 159143-50-7 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

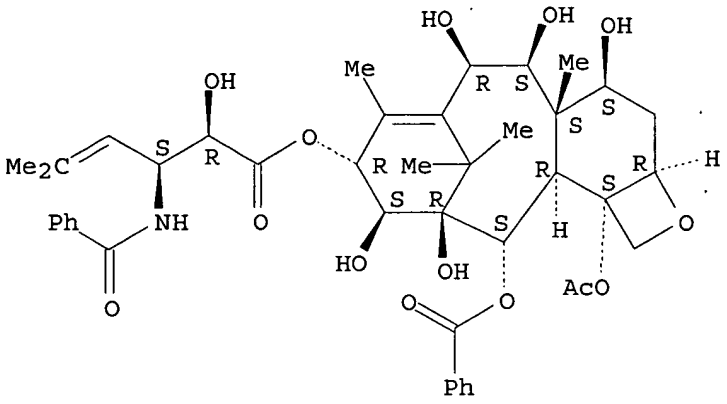
Absolute stereochemistry.



RN 185623-21-6 CAPLUS

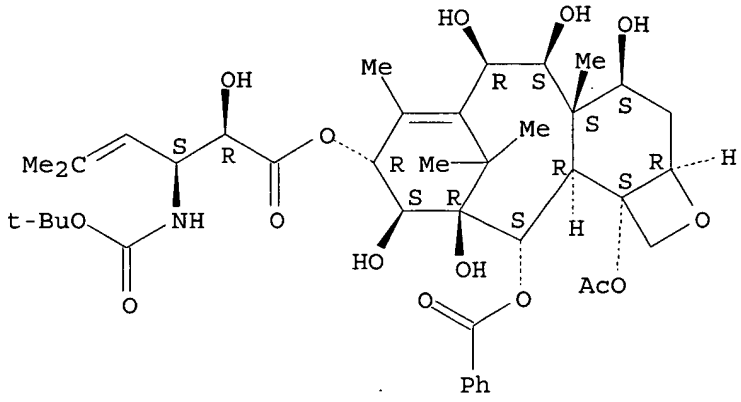
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



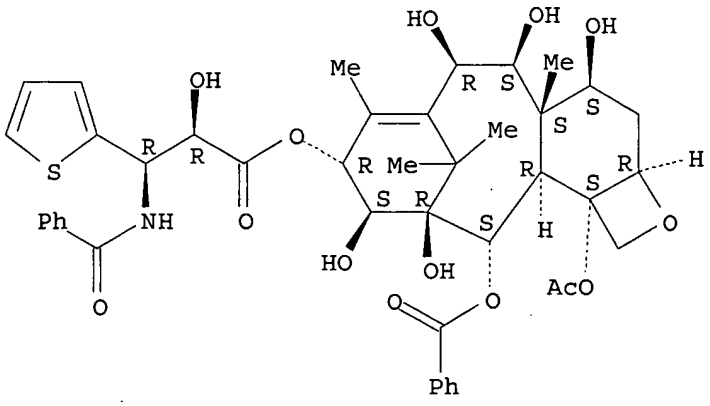
RN 232948-51-5 CAPLUS
CN 4-Hexenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



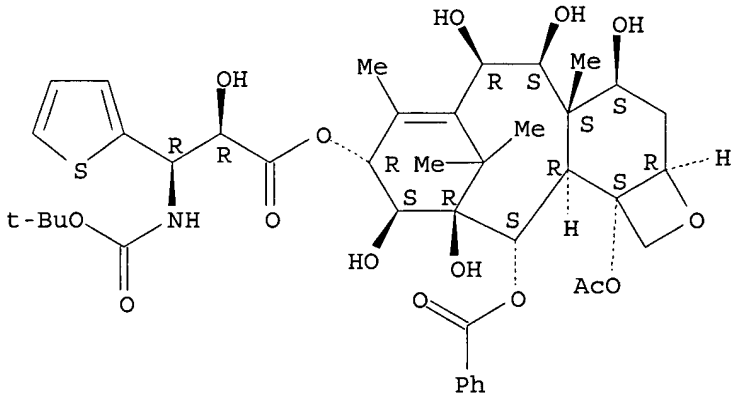
RN 232948-52-6 CAPLUS
CN 4-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



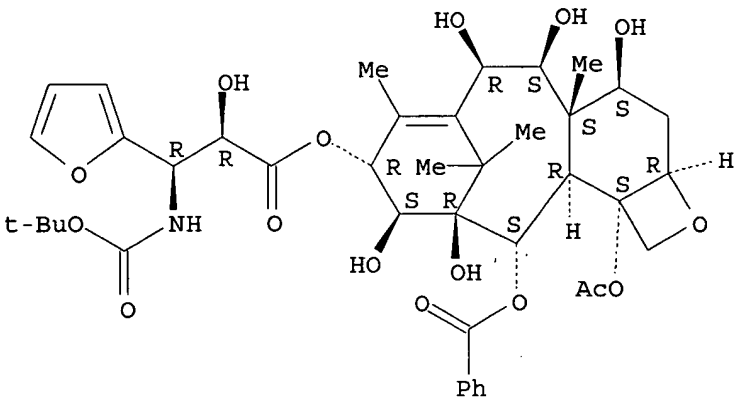
RN 232948-49-1 CAPLUS
CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



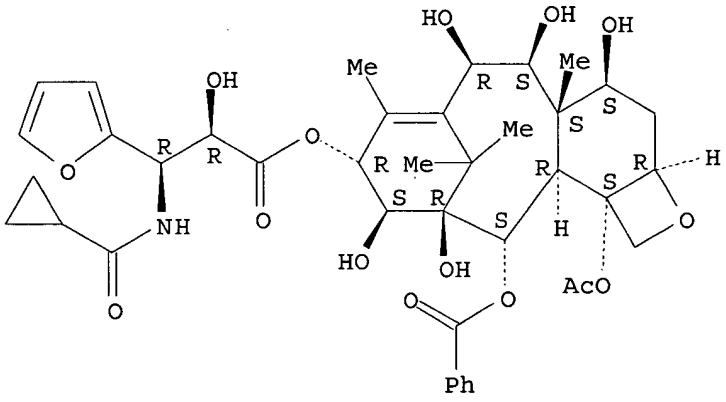
RN 232948-50-4 CAPLUS
CN 4-Hexenoic acid, 3-(benzoylamino)-2-hydroxy-5-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



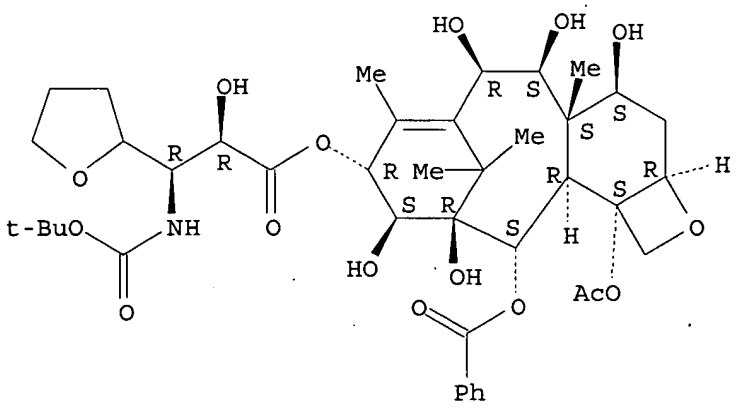
RN 232948-47-9 CAPLUS
CN 2-Furanpropanoic acid, β-[(cyclopropylcarbonyl)amino]-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



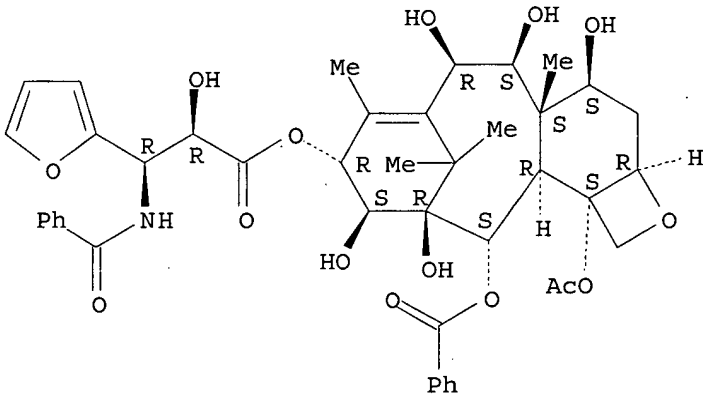
RN 232948-48-0 CAPLUS
CN 2-Thiophenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



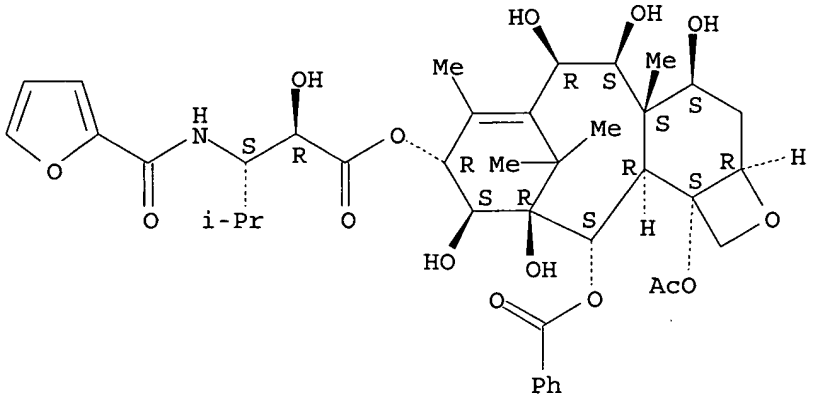
RN 232948-45-7 CAPLUS
CN 2-Furanpropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



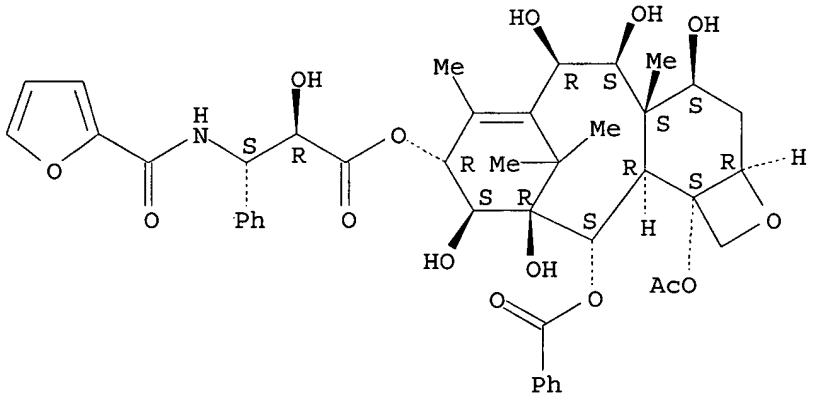
RN 232948-46-8 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



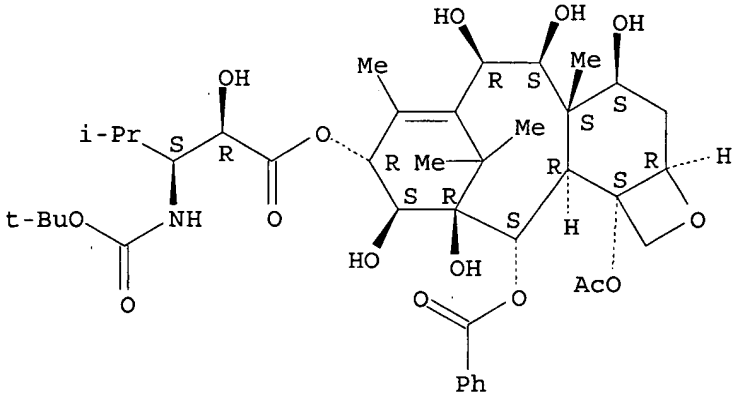
RN 232948-43-5 CAPLUS
CN Benzenepropanoic acid, β-[(2-furanylcarbonyl)amino]-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



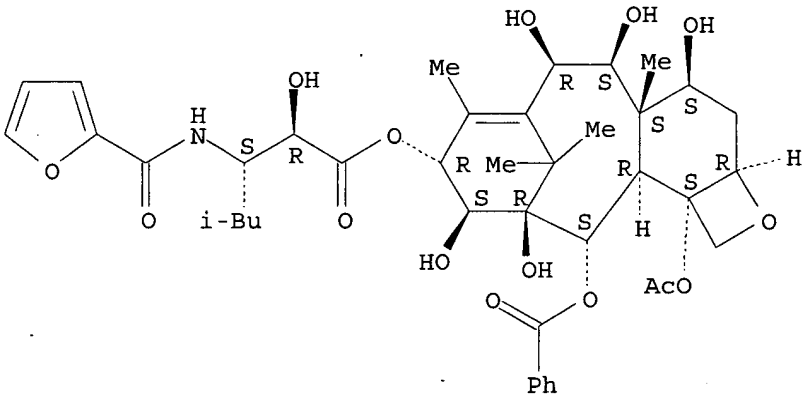
RN 232948-44-6 CAPLUS
CN L-threo-Heptonic acid, 4,7-anhydro-3,5,6-trideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (4ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



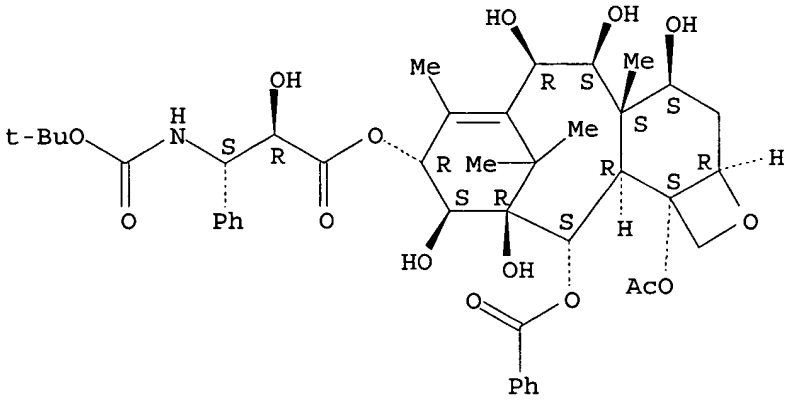
RN 232948-40-2 CAPLUS
CN Hexanoic acid, 3-[(2-furanylcarbonyl)amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



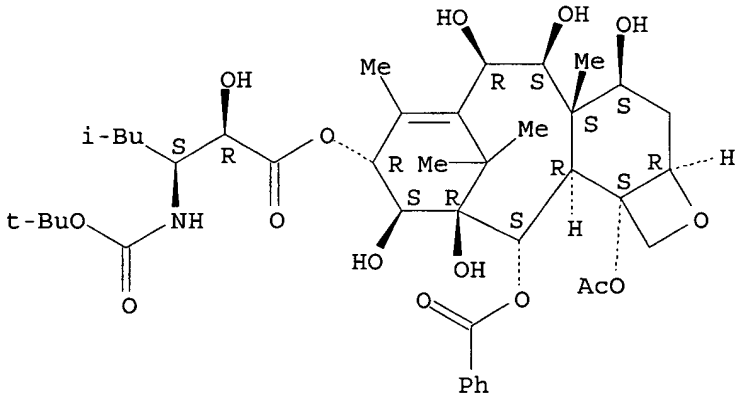
RN 232948-41-3 CAPLUS
CN L-threo-Pentonic acid, 3,4,5-trideoxy-3-[(2-furanylcarbonyl)amino]-4-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 232948-38-8 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

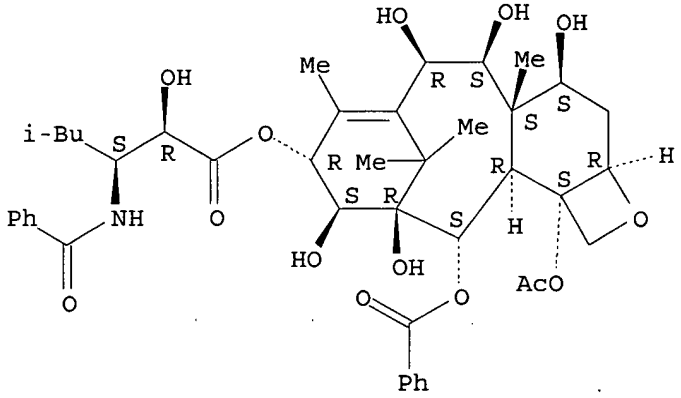


RN 232948-39-9 CAPLUS
CN L-threo-Pentonic acid, 3,4,5-trideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

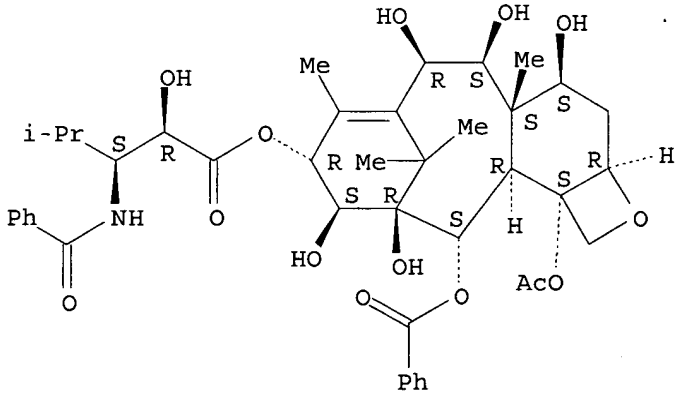
CN Hexanoic acid, 3-(benzoylamino)-2-hydroxy-5-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 232948-36-6 CAPLUS
CN L-threo-Pentonic acid, 3-(benzoylamino)-3,4,5-trideoxy-4-methyl-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 232948-37-7 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

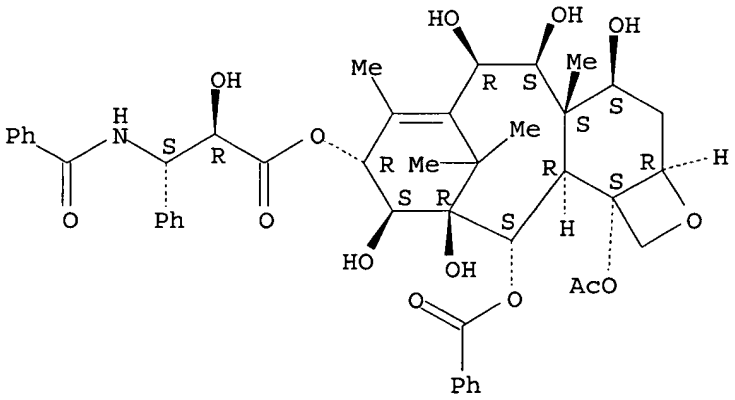
232948-58-2P 232948-59-3P 232948-60-6P 232948-61-7P 232948-62-8P
232948-63-9P 232948-64-0P 232948-65-1P 232948-66-2P 232948-67-3P
232948-68-4P 232948-69-5P 232948-70-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel water soluble taxane diterpenes as anticancer agents)

IT 1191-15-7, Diisobutylaluminum hydride 7784-21-6, Aluminum hydride 13813-25-7, Samarium iodide 16940-66-2, Sodium borohydride 16949-15-8, Lithium borohydride 25895-60-7, Sodium cyanoborohydride 33725-74-5, Tetrabutylammonium borohydride 156940-43-1 156940-44-2
159143-50-7 185623-21-6 186348-06-1 186348-08-3
186348-22-1 **232948-71-9 232948-72-0**
232948-74-2 232948-75-3 232948-76-4
232948-77-5 232948-78-6 232948-79-7
232948-80-0 232948-81-1 232948-82-2
232948-83-3 232948-84-4 232948-85-5
232948-86-6 232948-87-7 232948-88-8 232948-89-9
232948-90-2 232948-91-3 232948-92-4 232948-93-5 232948-94-6
232948-95-7 232948-96-8 232948-97-9 232948-98-0 232949-00-7
232949-01-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel water soluble taxane diterpenes as anticancer agents)

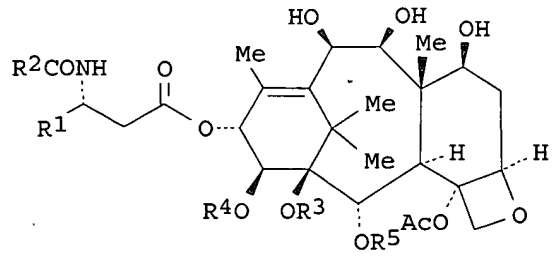
IT **232948-34-4P**, 10-Deacetyl-9-deketo-9β,14β-dihydroxypaclitaxel **232948-35-5P 232948-36-6P**
232948-37-7P 232948-38-8P 232948-39-9P
232948-40-2P 232948-41-3P 232948-43-5P
232948-44-6P 232948-45-7P 232948-46-8P
232948-47-9P 232948-48-0P 232948-49-1P
232948-50-4P 232948-51-5P 232948-52-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel water soluble taxane diterpenes as anticancer agents)

RN 232948-34-4 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,5S,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,6,10,11-pentahydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

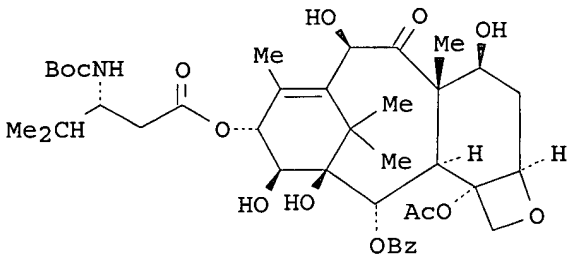
Absolute stereochemistry.



RN 232948-35-5 CAPLUS



I



II

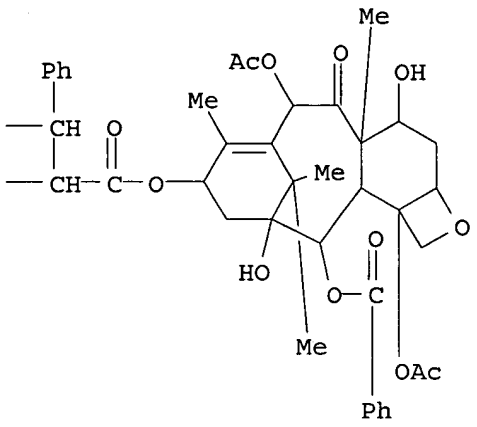
AB The present invention relates to novel taxane terpene compds. I [R1 = (un)substituted, straight or branched alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, cycloalkenyl or heterocycloalkenyl; R2 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, cycloalkenyl, heterocycloalkenyl, aryl or heteroaryl, RO-, RS- or RR6N-; R = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, cycloalkenyl, heterocycloalkenyl, aryl or heteroaryl; R6 = H, R; RR6 together form a cyclic structure; R3 = H, acyl, alkyl, alkenyl, alkynyl, (un)substituted cycloalkyl, heterocycloalkyl, cycloalkenyl, heterocycloalkenyl, aryl, heteroaryl or a hydroxy protecting group; R4 = H, acyl, alkyl, alkenyl, alkynyl, (un)substituted cycloalkyl, heterocycloalkyl, cycloalkenyl, heterocycloalkenyl, aryl, heteroaryl, or a hydroxy protecting group; R3R4 together form cyclic carbonate, cyclic thiocarbonate or acetonide structure; R5 = aryl] useful as anti-cancer agents and to a process for preparing I. Thus, I (R1 = CHMe2, R2 = OCMe3, R3 = R4 = H, R5 = Ph) was prepared in 75% yield via reduction of 10-deacetyl-14β-hydroxypaclitaxel (II) with samarium iodide in aqueous THF. I (R1 = CHMe2, R2 = OCMe3, R3 = R4 = H, R5 = Ph) was tested for water solubility (0.2214 mg/mL) and antitumor activity [ED50(test compound)/ED50(paclitaxel) = 4 (A549 cancer cell line); ED50(test compound)/ED50(paclitaxel) = 8.2 (SKOV-3 cancer cell line); ED50(test compound)/ED50(paclitaxel) = 5.5 (SK-MEL-2 cancer cell line); ED50(test compound)/ED50(paclitaxel) = 3.1 (HCT15 cancer cell line); ED50(test compound)/ED50(paclitaxel) = 1.0 (XF498 cancer cell line)].

IC ICM C07D305-14

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

IT 33069-62-4DP, Paclitaxel, analogs 114977-28-5DP, Docetaxel, analogs **232948-34-4P**, 10-Deacetyl-9-deketo-9β,14β-dihydroxypaclitaxel **232948-35-5P 232948-36-6P 232948-37-7P 232948-38-8P 232948-39-9P 232948-40-2P 232948-41-3P 232948-43-5P 232948-44-6P 232948-45-7P 232948-46-8P 232948-47-9P 232948-48-0P 232948-49-1P 232948-50-4P 232948-51-5P 232948-52-6P** 232948-53-7P 232948-54-8P 232948-55-9P 232948-56-0P 232948-57-1P

PAGE 1-B



L54 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:487282 CAPLUS
DOCUMENT NUMBER: 131:116387
TITLE: Preparation of novel water soluble taxane diterpenes as anticancer agents
INVENTOR(S): Chai, Ki Byung; Moon, Young Ho; Kim, Nam Du; Ha, Tae Hee; Shin, Jung Ae; Lim, Chang Gi; Kim, Wan Joo; Lee, Gwan Sun; Suh, Kwee Hyun
PATENT ASSIGNEE(S): Hanmi Pharmaceutical Co., Ltd., S. Korea
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9937631	A1	19990729	WO 1999-KR39		19990125
W: AU, CA, CN, JP, RU, US					
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
AU 9921877	A1	19990809	AU 1999-21877		19990125
PRIORITY APPLN. INFO.:			KR 1998-2430	A	19980126
			WO 1999-KR39	W	19990125

OTHER SOURCE(S): CASREACT 131:116387; MARPAT 131:116387
GI

animals. Thus, steroid-containing macrolide glycopeptide I was prepared as as carriers for steroid/non-steroid anti-inflammatory, antineoplastic, and antiviral active mol. The compds. demonstrating a 30% or higher inhibition of TNF-α production at a dose of 10 mg/kg are considered active. The compds. demonstrating the same or better analgesic activity in mice than acetyl salicylic acid are considered active. In vitro assay for antineoplastic activity and inhibitory effect on HIV replication are reported.

IC ICM C07J

CC 33-7 (Carbohydrates)
Section cross-reference(s): 1, 32, 34, 63

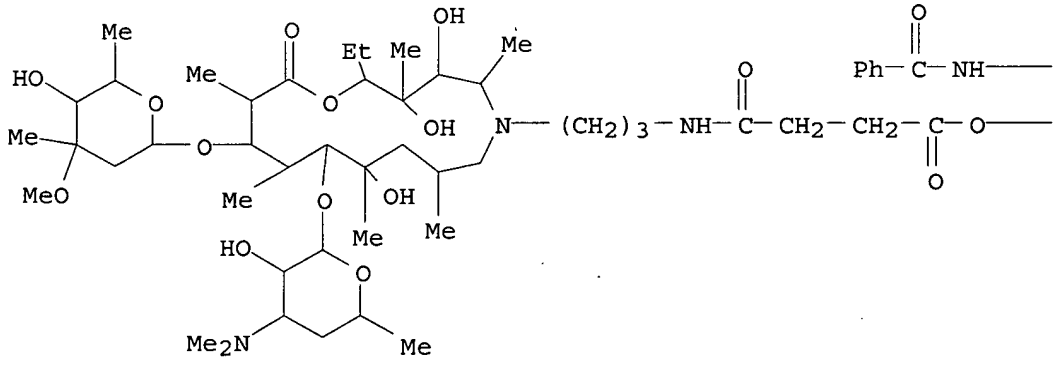
IT 641630-46-8P 641630-48-0P 641630-49-1P 641630-50-4P 641630-51-5P
641630-52-6P 641630-53-7P 641630-54-8P 641630-55-9P 641630-56-0P
641630-57-1P 641630-58-2P 641630-59-3P 641630-60-6P 641630-61-7P
641630-62-8P 641630-63-9P 641630-64-0P **641630-65-1P**
641630-66-2P 641630-67-3P 642087-21-6P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroid-containing macrolide glycopeptides as carriers for steroid/non-steroid anti-inflammatory, antineoplastic, and antiviral active mols.)

IT **641630-65-1P**
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroid-containing macrolide glycopeptides as carriers for steroid/non-steroid anti-inflammatory, antineoplastic, and antiviral active mols.)

RN 641630-65-1 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-[4-[[3-[(2R,3S,4R,5R,8R,10R,11R,12S,13S,14R)-13-[(2,6-dideoxy-3-C-methyl-3-O-methyl-α-L-ribo-hexopyranosyl)oxy]-2-ethyl-3,4,10-trihydroxy-3,5,8,10,12,14-hexamethyl-15-oxo-11-[[3,4,6-trideoxy-3-(dimethylamino)-β-D-xylo-hexopyranosyl]oxy]-1-oxa-6-azacyclopentadec-6-yl]propyl]amino]-1,4-dioxobutoxy]-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-3,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

PAGE 1-A

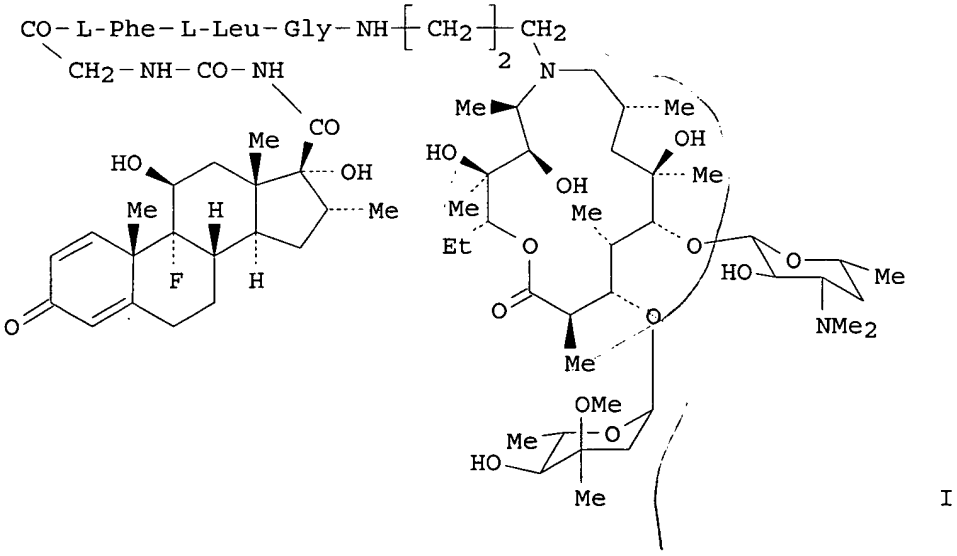


PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005313	A2	20040115	WO 2003-IB3792	20030708
WO 2004005313	A3	20050421		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003264917	A1	20040123	AU 2003-264917	20030708
US 2004077612	A1	20040422	US 2003-616046	20030708
EP 1551865	A2	20050713	EP 2003-762853	20030708
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1665831	A	20050907	CN 2003-816097	20030708
JP 2005538070	T2	20051215	JP 2004-519131	20030708
NO 2005000575	A	20050315	NO 2005-575	20050202
PRIORITY APPLN. INFO.:			US 2002-395190P P	20020708
			WO 2003-IB3792 W	20030708

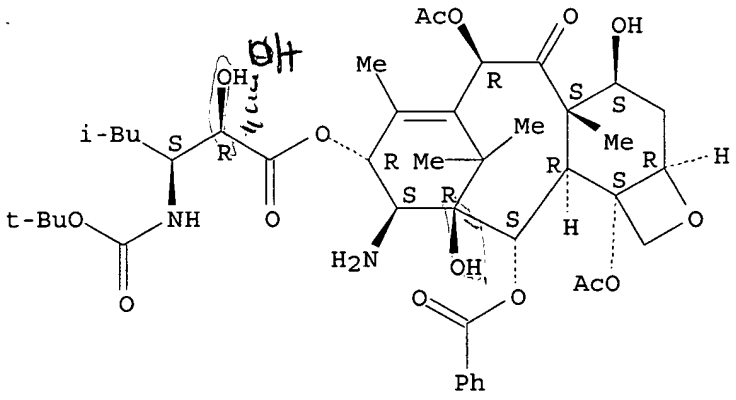
OTHER SOURCE(S): MARPAT 140:94230

GI



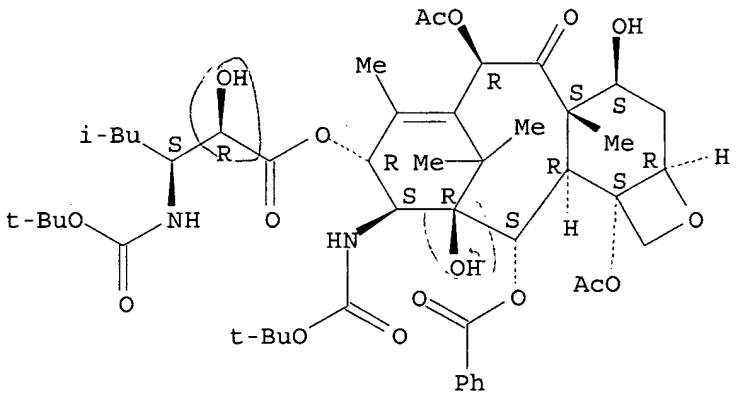
I

AB The present invention relates (a) to new compds. represented by formula M-L-V; wherein M represents a macrolide moiety derived from macrolide possessing the property of accumulation in inflammatory cells, V represents and ant-inflammatory steroid or nonsteroid subunit, or an antineoplastic or antiviral subunit and L represents a linking group covalently linking M and V; (b) to their pharmacol. acceptable salts, prodrugs and solvates, (c) to processes and intermediates for their preparation, and (d) to their use in the treatment of inflammatory/neoplastic/viral diseases and conditions in humans and



RN 675584-63-1 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-10-[[(1,1-dimethylethoxy)carbonyl]amino]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L54 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:41493 CAPLUS
DOCUMENT NUMBER: 140:94230
TITLE: Preparation of steroid-containing macrolide glycopeptides as carriers for steroid/non-steroid anti-inflammatory, antineoplastic, and antiviral active molecules
INVENTOR(S): Mercep, Mladen; Mesic, Milan; Tomaskovic, Linda; Markovic, Stribor
PATENT ASSIGNEE(S): Pliva D.D., Croatia; Pliva - Istrazivacki Institut D.O.O.
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

acyl, hydroxyaminoacyl], from 13-ketobaccatin derivs. II via functionalization at the 14-position. Thus, preparation of taxane derivative I [XR4 = NHCO; R1 = TES; R2 = Ac; R6 = C6H5; R9 = H] was achieved via a multistep synthetic sequence starting from II (R1 = H; R2 = Ac, R4 = H; R6 = C6H5).

IC ICM C07D305-14

CC 30-20 (Terpenes and Terpenoids)

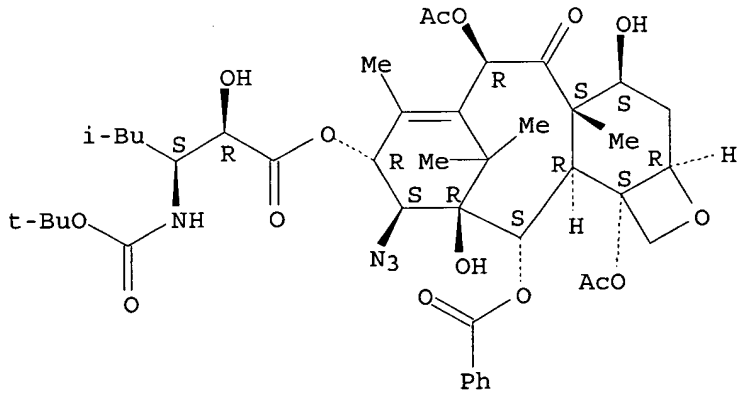
IT 675584-48-2P 675584-49-3P 675584-51-7P **675584-54-0P**
675584-59-5P **675584-61-9P 675584-63-1P** 675584-65-3P
675584-66-4P 675584-67-5P 675584-68-6P 675584-69-7P 675584-70-0P
675584-71-1P 675584-73-3P 675584-76-6P 675584-77-7P 675584-78-8P
675584-79-9P 675584-80-2P 675584-81-3P 675584-82-4P 675584-83-5P
675584-88-0P 675584-89-1P 675584-90-4P 675584-91-5P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of taxane derivs. functionalized at the 14-position)

IT **675584-54-0P 675584-61-9P 675584-63-1P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of taxane derivs. functionalized at the 14-position)

RN 675584-54-0 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-6,12b-bis(acetyloxy)-10-azido-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 675584-61-9 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-6,12b-bis(acetyloxy)-10-amino-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

functionalized at the 14-position

INVENTOR(S): Fontana, Gabriele; Bombardelli, Ezio; Battaglia, Arturo; Baldelli, Eleonora; Guerrini, Andrea; Gelmi, Maria Luisa; Carenzi, Giacomo; Pocar, Donato

PATENT ASSIGNEE(S): Indena S.P.A., Italy

SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

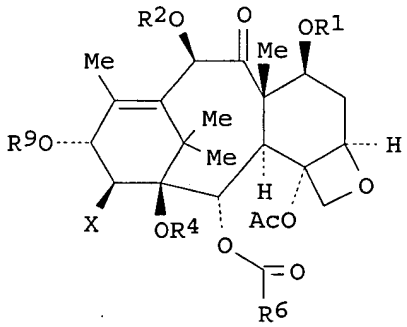
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024706	A2	20040325	WO 2003-EP9866	20030905
WO 2004024706	A3	20040708		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2498277	AA	20040325	CA 2003-2498277	20030905
AU 2003267049	A1	20040430	AU 2003-267049	20030905
EP 1537093	A2	20050608	EP 2003-747971	20030905
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1681799	A	20051012	CN 2003-821338	20030905
JP 2006503030	T2	20060126	JP 2004-535440	20030905
NO 2005001774	A	20050510	NO 2005-1774	20050411
US 2006122258	A1	20060608	US 2005-527164	20051109

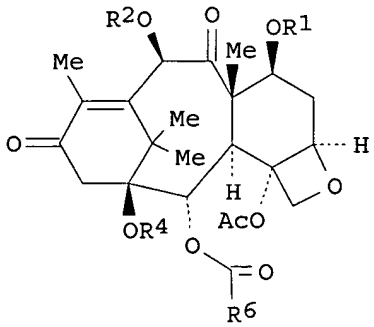
PRIORITY APPLN. INFO.: IT 2002-MI1921 A 20020910
WO 2003-EP9866 W 20030905

OTHER SOURCE(S): MARPAT 140:287557

GI



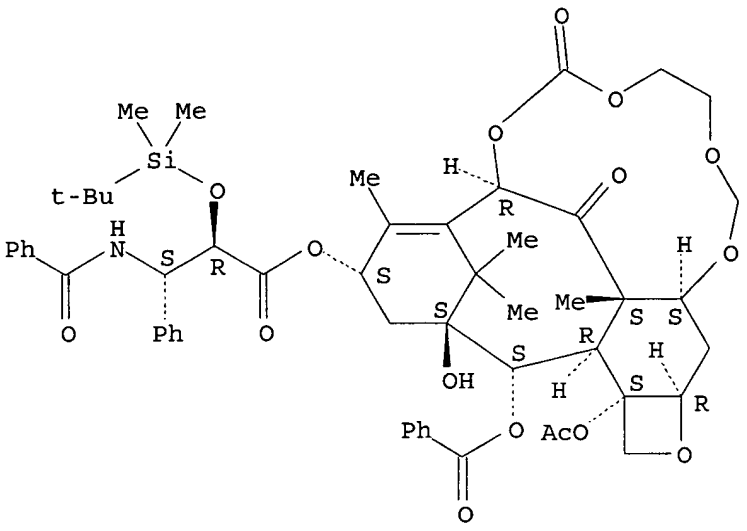
I



II

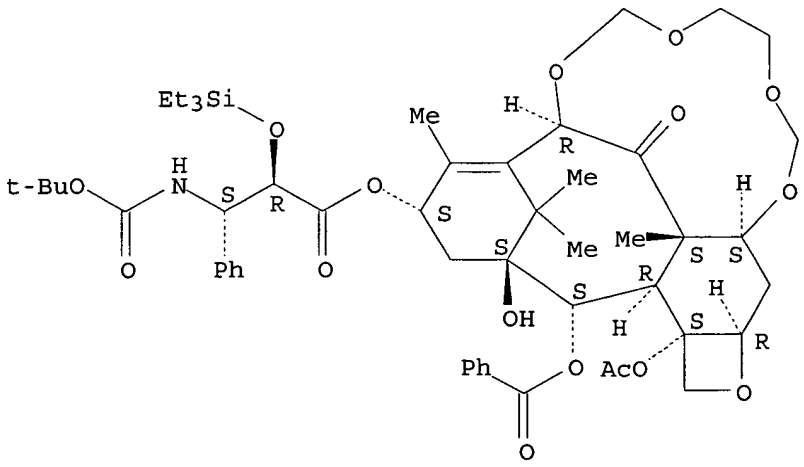
AB The present invention discloses a general process for the preparation of taxane derivs. such as I [X = N3, NH2, NHR3, :CHR8, OR3; R1 = H, protecting groups; R2 = H, acyl; R3 = alkoxycarbonyl; R3R4 = CO, CS, SO, SO2; R4 = H; R6 = aryl, heteroaryl; R8 = H, alkyl, alkoxycarbonyl; R4R8 = CO; R9 =

Absolute stereochemistry.



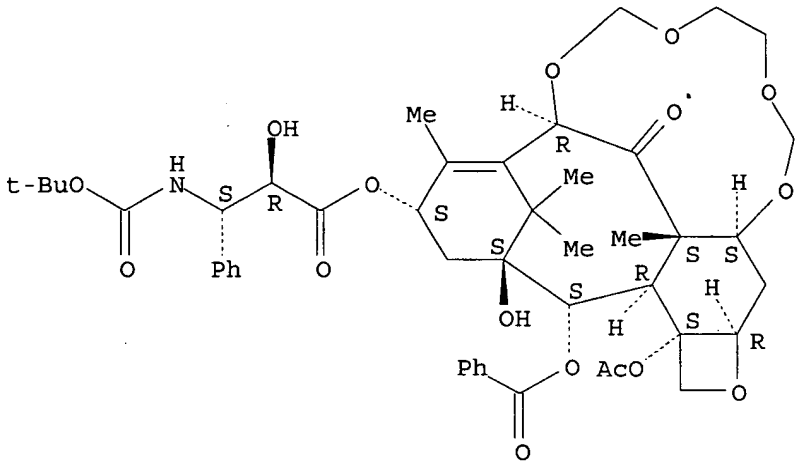
RN 709673-81-4 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, (9R,10aS,11R,11aS,13aR,14aS,15S,16S,20S)-11a-(acetyloxy)-15-(benzoyloxy)-4,5,9,10,10a,11a,12,13a,14,14a,16,17,20,21-tetradecahydro-16-hydroxy-10a,17,17,19-tetramethyl-10-oxo-9,11-([1,3]benzenomethano)-11H-oxeto[3,2-m]-1,3,6,8-benzotetraoxacyclododecin-20-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



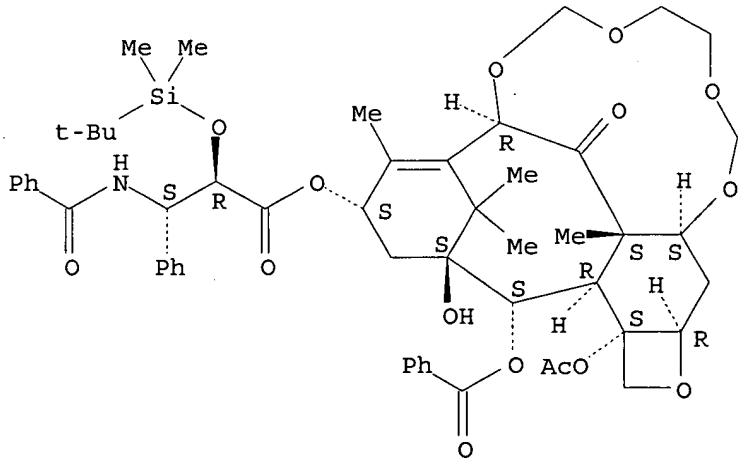
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:252495 CAPLUS
DOCUMENT NUMBER: 140:287557
TITLE: Process for preparation of taxane derivatives

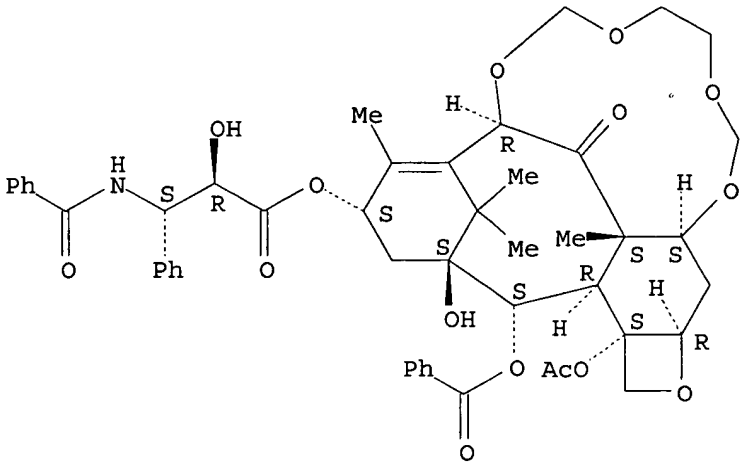


IT **709673-66-5P 709673-78-9P 709673-81-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. activity of macrocyclic taxane analogs)
RN 709673-66-5 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (9R,10aS,11R,11aS,13aR,14aS,15S,16S,20S)-11a-(acetyloxy)-15-(benzoyloxy)-4,5,9,10,10a,11a,12,13a,14,14a,16,17,20,21-tetradecahydro-16-hydroxy-10a,17,17,19-tetramethyl-10-oxo-9,11-([1,3]benzenomethano)-11H-oxeto[3,2-m]-1,3,6,8-benzotetraoxacyclododecin-20-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

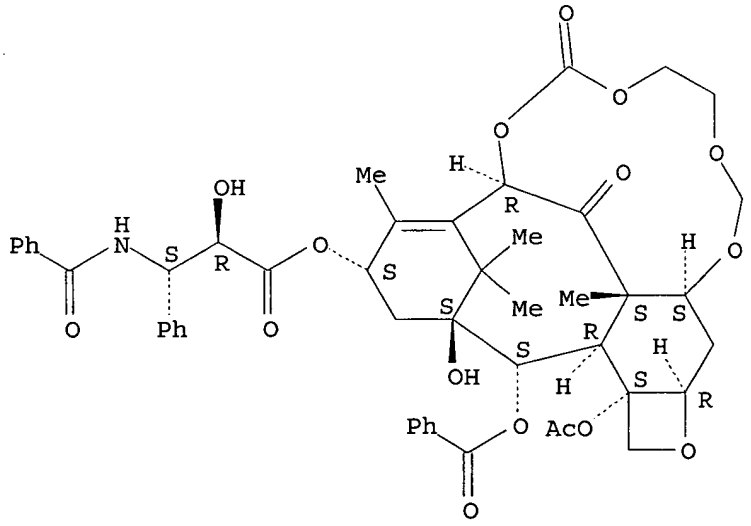


RN 709673-78-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (9R,10aS,11R,11aS,13aR,14aS,15S,16S,20S)-11a-(acetyloxy)-15-(benzoyloxy)-4,5,9,10,10a,11a,12,13a,14,14a,16,17,20,21-tetradecahydro-16-hydroxy-10a,17,17,19-tetramethyl-7,10-dioxo-9,11-([1,3]benzenomethano)-11H-oxeto[3,2-m]-1,3,6,8-benzotetraoxacyclododecin-20-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)



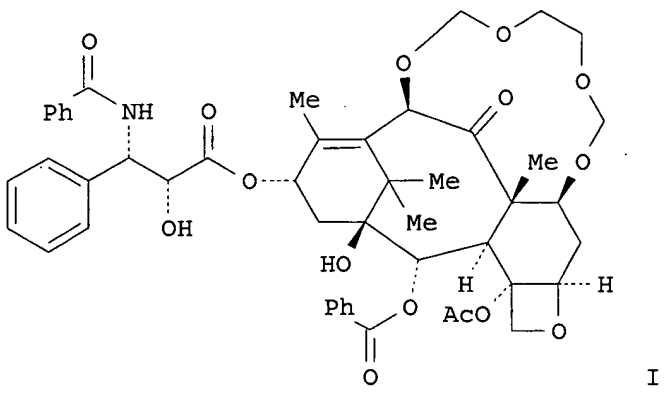
RN 709673-73-4 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (9R,10aS,11R,11aS,13aR,14aS,15S,16S,20S)-11a-(acetyloxy)-15-(benzoyloxy)-4,5,9,10,10a,11a,12,13a,14,14a,16,17,20,21-tetradecahydro-16-hydroxy-10a,17,17,19-tetramethyl-7,10-dioxo-9,11-([1,3]benzenomethano)-11H-oxeto[3,2-m]-1,3,6,8-benzotetraoxacyclododecin-20-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 709673-76-7 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (9R,10aS,11R,11aS,13aR,14aS,15S,16S,20S)-11a-(acetyloxy)-15-(benzoyloxy)-4,5,9,10,10a,11a,12,13a,14,14a,16,17,20,21-tetradecahydro-16-hydroxy-10a,17,17,19-tetramethyl-10-oxo-9,11-([1,3]benzenomethano)-11H-oxeto[3,2-m]-1,3,6,8-benzotetraoxacyclododecin-20-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



I

AB A series of paclitaxel analogs, e.g. I, possessing a macrocyclic structure between the 7 and 10 positions has been prepared These compds. possess in vitro activity against a paclitaxel resistant cell line and have in vivo activity comparable to paclitaxel.

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

IT **709673-71-2P 709673-73-4P 709673-76-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. activity of macrocyclic taxane analogs)

IT 114655-02-6P 162375-26-0P 709673-63-2P **709673-66-5P**
709673-69-8P 709673-74-5P 709673-75-6P **709673-78-9P**
709673-79-0P 709673-80-3P **709673-81-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. activity of macrocyclic taxane analogs)

IT **709673-71-2P 709673-73-4P 709673-76-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. activity of macrocyclic taxane analogs)

RN 709673-71-2 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (9R,10aS,11R,11aS,13aR,14aS,15S,16S,20S)-11a-(acetyloxy)-15-(benzoyloxy)-4,5,9,10,10a,11a,12,13a,14,14a,16,17,20,21-tetradecahydro-16-hydroxy-10a,17,17,19-tetramethyl-10-oxo-9,11-([1,3]benzenomethano)-11H-oxeto[3,2-m]-1,3,6,8-benzotetraoxacyclododecin-20-yl ester, (αR,βS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

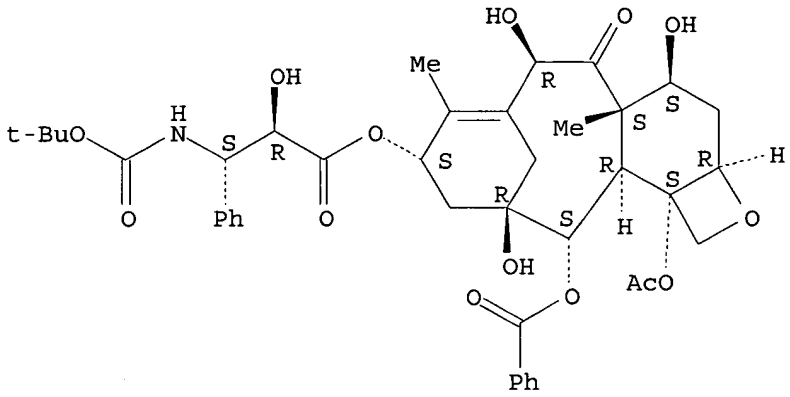
794517-81-0 794517-82-1 794517-83-2 794517-84-3 794517-85-4
794517-87-6 794517-88-7 794517-90-1 **794517-91-2**
794517-92-3 794517-93-4 794517-94-5 794517-95-6 794517-96-7
794517-97-8 794517-98-9 795297-26-6, AG 1132 795297-28-8
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(incorporating protein flexibility in structure-based drug discovery using HIV-1 protease as a test case)

IT **794517-91-2**
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(incorporating protein flexibility in structure-based drug discovery using HIV-1 protease as a test case)

RN 794517-91-2 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8-dimethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:346260 CAPLUS
DOCUMENT NUMBER: 141:71731
TITLE: Synthesis and biological activity of macrocyclic taxane analogues
AUTHOR(S): Tarrant, James G.; Cook, Donald; Fairchild, Craig; Kadow, John F.; Long, Byron H.; Rose, William C.; Vyas, Dolatrai
CORPORATE SOURCE: Discovery Chemistry, Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492-7660, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2555-2558
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:71731
GI

AUTHOR(S): Meagher, Kristin L.; Carlson, Heather A.
CORPORATE SOURCE: College of Pharmacy, Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI, 48109-1065, USA
SOURCE: Journal of the American Chemical Society (2004), 126(41), 13276-13281
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have developed a receptor-based pharmacophore method which utilizes a collection of protein structures to account for inherent protein flexibility in structure-based drug design. Several procedures were systematically evaluated to derive the most general protocol for using multiple protein structures. Most notably, incorporating more protein flexibility improved the performance of the method. The pharmacophore models successfully discriminate known inhibitors from drug-like non-inhibitors. Furthermore, the models correctly identify the bound conformations of some ligands. We used unliganded HIV-1 protease to develop and validate this method. Drug design is always initiated with a protein-ligand structure, and such success with unbound protein structures is remarkable - particularly in the case of HIV-1 protease, which has a large conformational change upon binding. This technique holds the promise of successful computer-based drug design before bound crystal structures are even discovered, which can mean a jump-start of 1-3 yr in tackling some medically relevant systems with computational methods.
CC 1-3 (Pharmacology)
IT 54-62-6 81-11-8 436-05-5, MCMC 10271 865-04-3 865-21-4, Vinblastine 1404-15-5 1461-15-0 1947-37-1, 4-7-Cholecystokinin-7 (swine) 2667-89-2 3785-44-2 6377-18-0 6998-60-3, Rifamycin 7488-76-8 10236-47-2 11076-29-2 15599-51-6, MCMC 2885 15964-31-5 22112-79-4 23412-26-2 29883-15-6 30658-43-6 31770-79-3, MCMC 3588 33605-67-3 34941-71-4 36980-34-4 38716-28-8, MCMC 6171 41600-33-3 49620-13-5 52196-22-2 54083-22-6, MCMC 4222 54138-84-0 56079-81-3 58761-87-8 66211-92-5, MCMC 4777 69414-41-1 69558-55-0 69866-21-3, MCMC 10279 70774-25-3 72559-06-9 78995-72-9 80394-65-6, MCMC 10434 84412-94-2 84799-23-5 85807-48-3 88391-91-7, MCMC 7748 93205-34-6 94168-98-6, MCMC 10469 97068-30-9 97275-40-6 103177-37-3 103336-05-6, MCMC 6317 108852-90-0 110417-88-4 110816-79-0 111902-57-9 112190-24-6 113786-33-7 117091-64-2 123524-52-7 125552-93-4 126333-28-6 126438-22-0 126456-36-8 127231-42-9 127779-20-8, Saquinavir 129467-45-4 129981-36-8 136679-36-2 137755-25-0 137882-98-5 140196-60-7, P9941 140703-51-1 141197-75-3 141396-10-3 141626-36-0 142694-73-3 143631-62-3 144412-49-7 144849-63-8 145040-37-5 145216-43-9 147318-81-8 148270-86-4 148314-61-8, LY289612 148504-51-2 148982-38-1 148993-96-8 150176-80-0 150322-97-7 150348-92-8 150378-17-9 150654-53-8 151581-24-7 152943-74-3 153026-04-1, L-700497 153183-11-0 153314-43-3 154612-31-4 155213-67-5 157999-29-6 159989-64-7 161302-38-1, BMS-182193 161814-49-9 161897-65-0 162168-92-5 163020-88-0 163462-08-6 163462-10-0 163633-45-2, AG 1254 164514-54-9 166186-75-0 166281-58-9 166335-18-8 169941-92-8 171435-79-3 171858-52-9 173261-21-7 173937-91-2 174391-92-5 174590-26-2 178471-24-4 180077-76-3 180077-78-5 180078-07-3 180283-41-4 181038-55-1 183321-74-6 183854-24-2 185449-98-3 192725-17-0, Lopinavir 203244-81-9 203244-82-0 213895-66-0 216103-83-2 216863-66-0 245125-93-3 413621-09-7 573987-37-8 573987-39-0 714192-77-5 760215-78-9 794517-69-4 794517-70-7 794517-71-8 794517-72-9 794517-73-0 794517-74-1 794517-75-2 794517-76-3 794517-77-4 794517-78-5 794517-79-6 794517-80-9

850498-78-1 850498-80-5 850498-82-7 850498-84-9 850498-86-1
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850499-49-9 850499-50-2 850499-51-3 850499-52-4 850499-53-5
850499-54-6 850499-55-7 850499-56-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(increasing drug efficiency using conjugates containing drug moiety and linker and substrate for protein or lipid kinase)

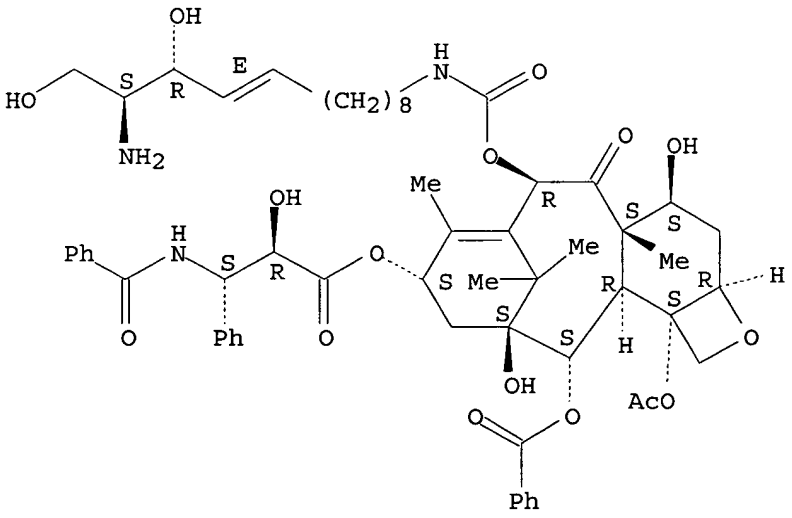
IT **850499-54-6**

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(increasing drug efficiency using conjugates containing drug moiety and linker and substrate for protein or lipid kinase)

RN 850499-54-6 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-6-[[[[(9E,11R,12S)-12-amino-11,13-dihydroxy-9-tridecenyl]amino]carbonyl]oxy]-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L54 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:783746 CAPLUS
DOCUMENT NUMBER: 141:420031
TITLE: Incorporating Protein Flexibility in Structure-Based Drug Discovery: Using HIV-1 Protease as a Test Case

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005035003	A2	20050421	WO 2004-US31148		20040922
WO 2005035003	A3	20050818			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 2005148534	A1	20050707	US 2004-948364		20040922
US 2005187147	A1	20050825	US 2004-948707		20040922
PRIORITY APPLN. INFO.:			US 2003-505325P	P	20030922
			US 2004-568340P	P	20040504
			US 2004-581835P	P	20040622
			US 2003-505033P	P	20030922

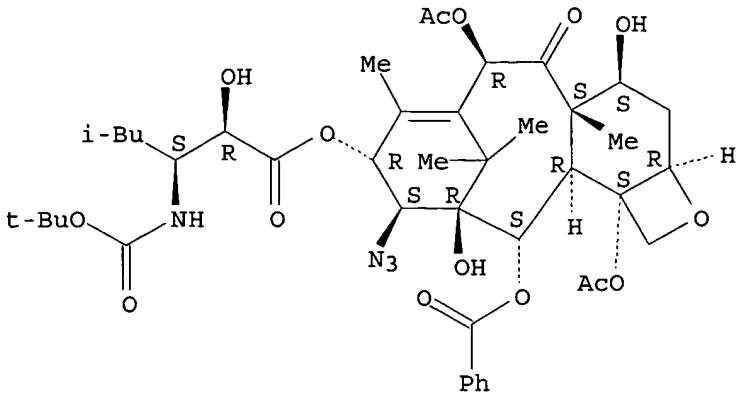
OTHER SOURCE(S): MARPAT 142:404292

AB In one embodiment, provided herein are compns. and methods for increasing drug efficiency. In certain embodiments, the compns. contain conjugates having the formula: D-L-S wherein D is a drug moiety; L, which may or may not be present, is a non-releasing linker moiety; and S is a substrate for a protein or lipid kinase that is overexpressed, overactive or exhibits undesired activity in a target system.

IC ICM A61K047-48
ICS C07K007-06; A61K038-08; A61P029-00; A61P035-00; A61K031-337; A61K031-475; A61K031-704

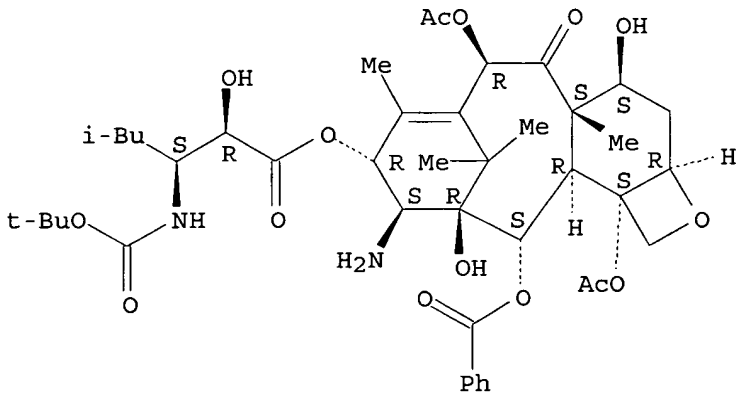
CC 1-12 (Pharmacology)
Section cross-reference(s): 34, 63

IT 50-07-7D, Mitomycin C, conjugates 50-18-0D, Cyclophosphamide, conjugates 50-44-2D, 6-Mercaptopurine, conjugates 51-21-8D, 5-Fluorouracil, conjugates 54-62-6D, Aminopterin, conjugates 57-22-7D, Vincristine, conjugates 59-05-2D, Methotrexate, conjugates 91-18-9D, Pteridine, derivs., conjugates 147-94-4D, Cytosine arabinoside, conjugates 148-82-3D, Melphalan, conjugates 518-28-5D, Podophyllotoxin, derivs., conjugates 528-74-5D, Dichloromethotrexate, conjugates 801-52-5D, Porfiromycin, conjugates 865-21-4, Vinblastine 1404-00-8D, Mitomycin, derivs., conjugates 2410-93-7D, Methopterin, conjugates 2998-57-4D, Estramustine, conjugates 3352-69-0D, 4-Desacetylvinblastine, conjugates 11056-06-7D, Bleomycin, derivs., conjugates 15228-71-4D, Leurosidine, conjugates 15663-27-1D, Cisplatin, conjugates 20830-81-3D, Daunorubicin, conjugates 23214-92-8D, Doxorubicin, derivs. 33069-62-4D, Paclitaxel, derivs. 33419-42-0D, Etoposide, conjugates 50935-04-1D, conjugates 53643-48-4D, Vindesine, conjugates 57103-68-1D, Maytansinol, conjugates 78432-77-6, 10-Desacetyl taxol 82855-09-2D, Combretastatin, conjugates 111372-15-7 114977-28-5D, Docetaxel, conjugates 117091-64-2D, Etoposide phosphate, conjugates 146307-39-3 152044-53-6D, Epothilone A, conjugates 152044-54-7D, Epothilone B, conjugates 220167-86-2 849206-51-5 849206-90-2 849206-91-3 849206-92-4 849206-93-5 849206-94-6 850497-99-3 850498-05-4 850498-07-6 850498-09-8 850498-11-2 850498-13-4 850498-15-6 850498-17-8 850498-19-0 850498-21-4 850498-27-0 850498-30-5 850498-33-8 850498-35-0 850498-37-2 850498-39-4 850498-41-8 850498-49-6 850498-51-0 850498-53-2 850498-55-4 850498-57-6 850498-59-8 850498-61-2 850498-63-4 850498-65-6 850498-67-8 850498-69-0 850498-71-4 850498-73-6 850498-76-9



RN 675584-61-9 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-6,12b-bis(acetyloxy)-10-amino-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

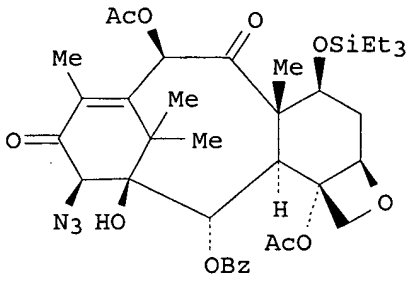
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:346897 CAPLUS
DOCUMENT NUMBER: 142:404292
TITLE: Compositions and methods for increasing drug efficiency
INVENTOR(S): Ballatore, Carlo; Castellino, Angelo John; Desharnais, Joel; Guo, Zijan; Li, Quing; Newman, Michael James; Sun, Chengzao
PATENT ASSIGNEE(S): Dihedron Corporation, USA
SOURCE: PCT Int. Appl., 404 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

"I.S.O.F.", Bologna, 40129, Italy
SOURCE: Tetrahedron (2005), 61(32), 7727-7745
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:248531
GI



I

AB The base induced deprotonation of H-14 of 7-triethylsilyl- (7-TES-) and 7-tert-butoxycarbonyl- (7-BOC-) protected 13-oxo-baccatins gave the corresponding enolates, which were selectively aminated with electrophilic nitrogen donors, such as azodicarboxylates and tosyl azide. In particular, tosyl azide gave the corresponding 7-BOC- and 7-TES-13-oxo-14β-azido-baccatin III. Alternatively, the last compound was prepared via NaN3 induced azidation of the 13-silyl enol ether of 7-TES-13-oxo-baccatin III under oxidative (cerium ammonium nitrate) conditions. The 13-silyl enol ether was obtained in a multistep process by DBU induced silylation of 7-TES-13-oxo-baccatin III. 7-TES-13-oxo-14β-azido-baccatin III (I) was used as a key intermediate for the synthesis of a new family of antitumor taxanes containing amino based functional groups at the C-14 position, such as: 14β-azido, 14β-amino, 14β-amino 1,14-carbamate, 14β-amino 1,14-thiocarbamate, and 14β-amino N-tert-butoxycarbonyl-1,14-carbamate.

CC 30-20 (Terpenes and Terpenoids)

IT 675584-48-2P 675584-49-3P 675584-51-7P **675584-54-0P**
675584-59-5P **675584-61-9P** 675584-65-3P 863489-80-9P
863489-81-0P 863489-82-1P 863489-83-2P 863489-84-3P 863489-87-6P
863489-88-7P 863489-90-1P 863489-91-2P 863489-93-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective synthesis of 14β-amino taxanes via stereoselective azidation)

IT **675584-54-0P 675584-61-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective synthesis of 14β-amino taxanes via stereoselective azidation)

RN 675584-54-0 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-6,12b-bis(acetyloxy)-10-azido-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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=> d stat que L54
L3                STR
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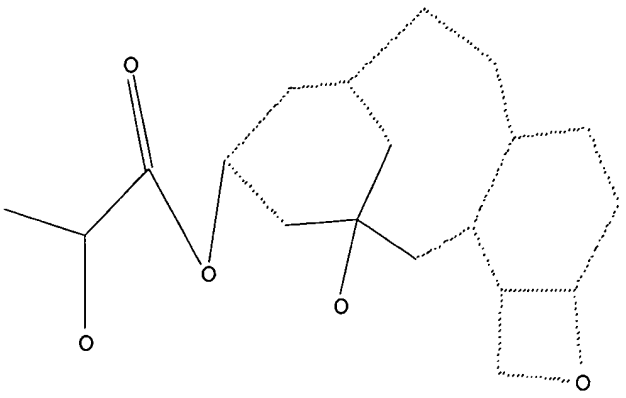

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L20               STR
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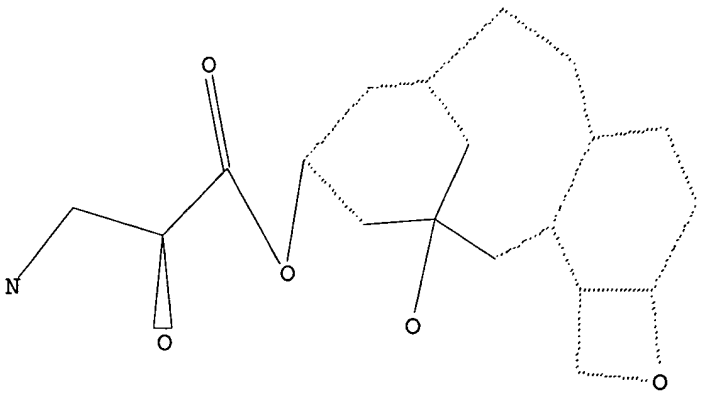

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L44           51 SEA FILE=REGISTRY ABB=ON  PLU=ON  11R AND L5
L45           14 SEA FILE=CAPLUS ABB=ON  PLU=ON  L44
L52            1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L45 AND L24
L54           13 SEA FILE=CAPLUS ABB=ON  PLU=ON  L45 NOT L52


=> d ibib abs hitind hitstr L54 1-13

L54  ANSWER 1 OF 13  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:589047  CAPLUS
DOCUMENT NUMBER:          143:248531
TITLE:                    Selective synthesis of 14β-amino taxanes
AUTHOR(S):                Battaglia, Arturo; Baldelli, Eleonora; Bombardelli,
                          Ezio; Carenzi, Giacomo; Fontana, Gabriele; Gelmi,
                          Maria Luisa; Guerrini, Andrea; Pocar, Donato
CORPORATE SOURCE:         Istituto CNR per la Sintesi Organica e Fotoreattivita
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STRUCTURE SEARCH #3

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=> file registry
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DICTIONARY FILE UPDATES:  18 SEP 2006  HIGHEST RN 907539-37-1

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

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FILE COVERS 1907 - 19 Sep 2006  VOL 145 ISS 13
FILE LAST UPDATED: 18 Sep 2006  (20060918/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html
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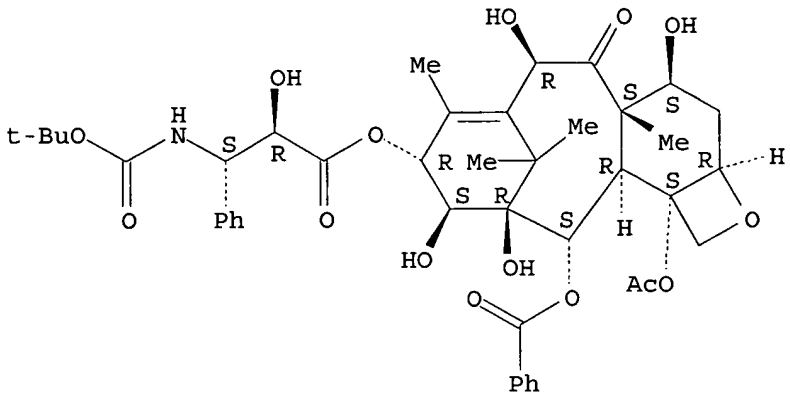
→ printed with structure search #2



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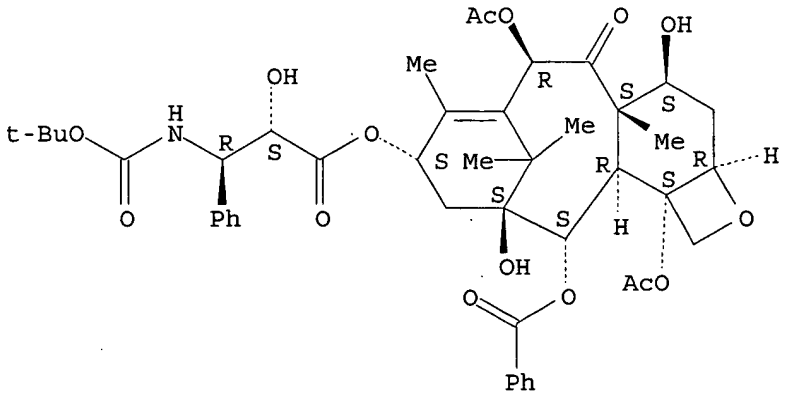
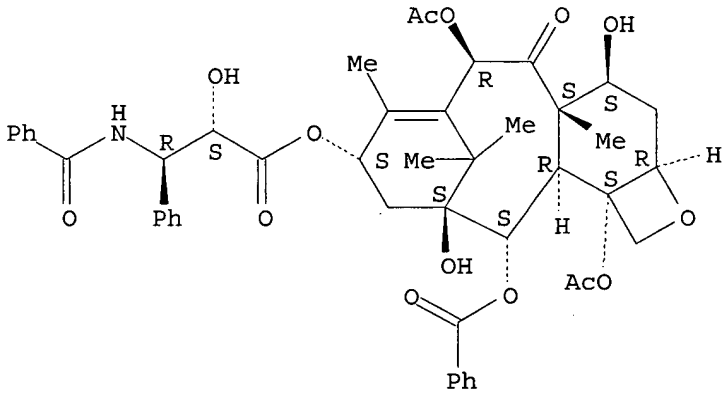


RN 149197-23-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159143-50-7 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9R,10S,11R,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,10,11-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

cross-validation r2cv of 0.640 and conventional r2 of 0.868. The predictive ability of training set model was tested on the test set of 14 compds. The tests not only revealed the robustness of the CoMFA model but demonstrated that for this model r2pred based on the mean activity of test set compds. can accurately estimate external predictivity but r2pred based on the mean activity of training set compds. overestimated the model. The CoMFA model explained why the activity of taxoid is sensitive to the stereochem. of the atoms at C-2' and C-3' positions and the presence of hydroxyl group at C-2' position. The other factors affecting activity were also elucidated according to standard coefficient contour maps of steric and electrostatic fields derived from the CoMFA model.

CC 1-3 (Pharmacology)
Section cross-reference(s): 22, 26

IT 33069-62-4 33069-62-4D, Paclitaxel, analogs 95603-46-6 110259-00-2
114977-28-5 114977-28-5D, Taxotere, analogs 114977-30-9 114977-31-0
125257-07-0 125354-16-7 **125354-17-8** 125354-18-9
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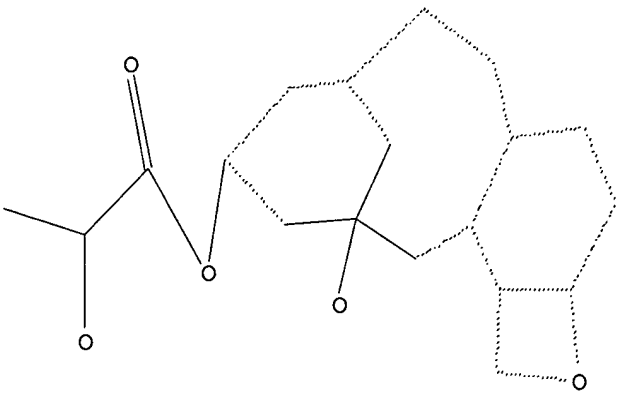
199657-71-1 199657-72-2 199657-73-3 199657-74-4 199657-75-5
199657-76-6 199737-26-3 199737-27-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(comparative mol. field anal. of paclitaxel analogs)

IT **125354-17-8 149197-23-9 159143-50-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(comparative mol. field anal. of paclitaxel analogs)

RN 125354-17-8 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L44 51 SEA FILE=REGISTRY ABB=ON PLU=ON 11R AND L5
L45 14 SEA FILE=CAPLUS ABB=ON PLU=ON L44

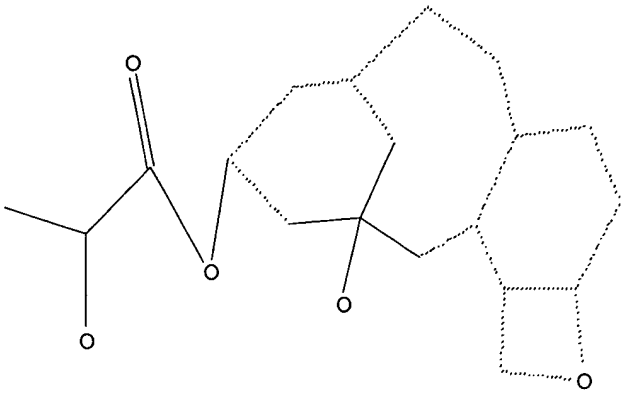
=> s L45 and L24
L52 1 L45 AND L24

=> s L45 and L24 and L49
L53 0 L45 AND L24 AND L49

=> d ibib abs hitind hitstr L52 1

L52 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:31653 CAPLUS
DOCUMENT NUMBER: 128:30043
TITLE: Comparative Molecular Field Analysis of A Series of Paclitaxel Analogs
AUTHOR(S): Zhu, Qiqing; Guo, Zongru; Huang, Niu; Wang, Minmin; Chu, Fengming
CORPORATE SOURCE: Department of Synthetic Medicinal Chemistry Institute of Materia Medica Chinese Academy of Medical Sciences, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Journal of Medicinal Chemistry (1997), 40(26), 4319-4328
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 94 paclitaxel analogs exhibiting antitumor activity by promoting the assembly of microtubules and inhibiting the disassembly process of microtubules to tubulin were investigated using the comparative mol. field anal. (CoMFA) method. These compds. belonging to 10 structural classes were randomly divided into a training set of 80 compds. and a test set of 14 compds. Since the 3-dimensional structure of ligand-receptor complex is unknown, from x-ray and NMR data, the authors rationally selected the 3-dimensional structure of paclitaxel in a polar solution as the active conformation and starting structure for mol. modeling, the other mols. were aligned using this mol. model as the template. The most optimal CoMFA yielded a 2-component model, with significant

L3 STR



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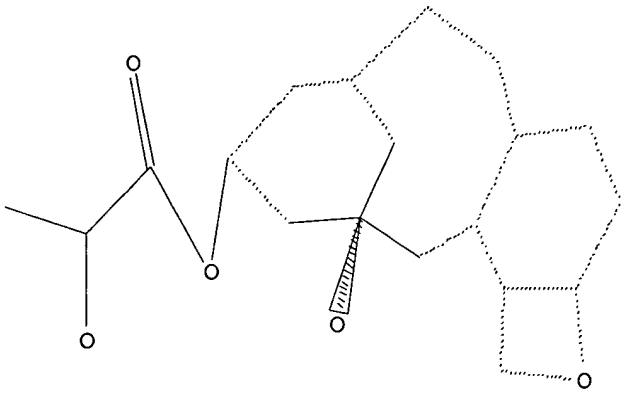
L14 STR



Structure attributes must be viewed using STN Express query preparation.
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SEARCH TIME: 00.00.01

=> d stat que L45
L3 STR

=> => □ STRUCTURE SEARCH #2

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DICTIONARY FILE UPDATES: 18 SEP 2006 HIGHEST RN 907539-37-1

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on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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FILE COVERS 1907 - 19 Sep 2006 VOL 145 ISS 13
FILE LAST UPDATED: 18 Sep 2006 (20060918/ED)

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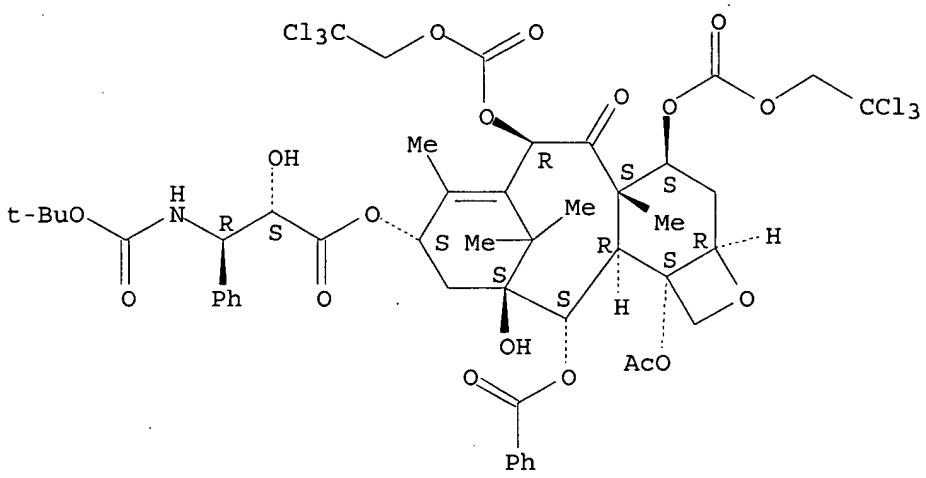
=> d stat que L16

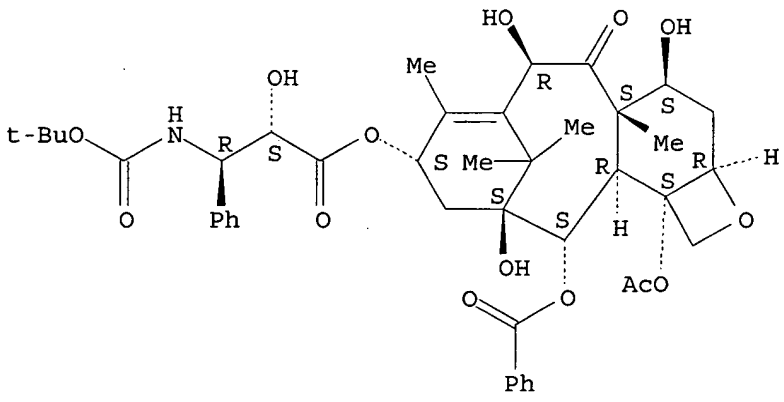
RN 114977-25-2 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **114977-29-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antitumor agent)
RN 114977-29-6 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

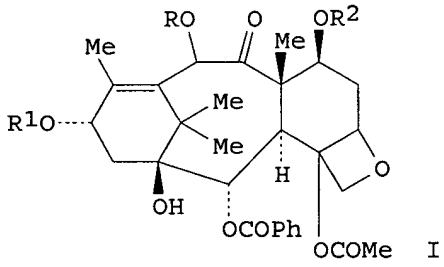
Absolute stereochemistry.



DOCUMENT NUMBER: 109:22762
TITLE: Preparation of taxol derivatives as antitumor agents
INVENTOR(S): Colin, Michel; Guenard, Daniel; Gueritte-Voegelein, Francoise; Potier, Pierre
PATENT ASSIGNEE(S): Rhone-Poulenc Sante, Fr.
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 253738	A1	19880120	EP 1987-401668		19870716
EP 253738	B1	19900131			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
FR 2601675	A1	19880122	FR 1986-10400		19860717
FR 2601675	B1	19880923			
US 4814470	A	19890321	US 1987-73156		19870714
AU 8775677	A1	19880121	AU 1987-75677		19870715
AU 591309	B2	19891130			
ZA 8705179	A	19880330	ZA 1987-5179		19870715
JP 63030479	A2	19880209	JP 1987-176071		19870716
JP 06051689	B4	19940706			
AT 49962	E	19900215	AT 1987-401668		19870716
CA 1278304	A1	19901227	CA 1987-542299		19870716
PRIORITY APPLN. INFO.:			FR 1986-10400	A	19860717
			EP 1987-401668	A	19870716

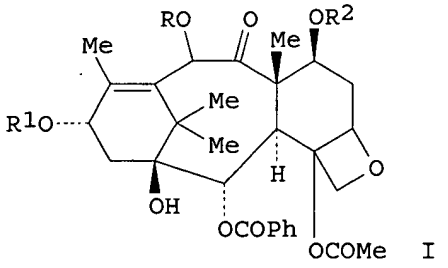
OTHER SOURCE(S): MARPAT 109:22762
GI



I

AB The title compds. (I; R = H, Ac; R1 = PhCHR4CHR3CO; R2 = H; 1 of R3, R4 = OH and the other = NHCO2CMe3) were prepared I (R = R1 = R2 = H) was stirred with ClCO2CH2CCl3 in pyridine to give I (R = R2 = CO2CH2CCl3, R1 = H) which was heated 18 h at 70° with PhCH:CHCO2H in PhMe containing DCC and dimethylaminopyridine to give I (R1 = trans-PhCH:CHCO, R, R2 as above). The latter was added to an MeCN solution of Me3CO2CNClNa (treated with AgNO3) and OsO4 and the mixture stirred 68 h in the dark with addnl. reagent addition to give I [R1 = (2'R,3'S)-COCH(OH)CHPhNHCO2CMe3, R, R2 as above] which was stirred 2 h in HOAc containing Zn to give I [R = R2 = H, R1 = (2'R,3'S)-COCH(OH)CHPhNHCO2CMe3]. At 1-10 mg/kg i.p. I are active in mice inoculated with L1210 or P388 leukemia.

IT **114977-25-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor agents)



I

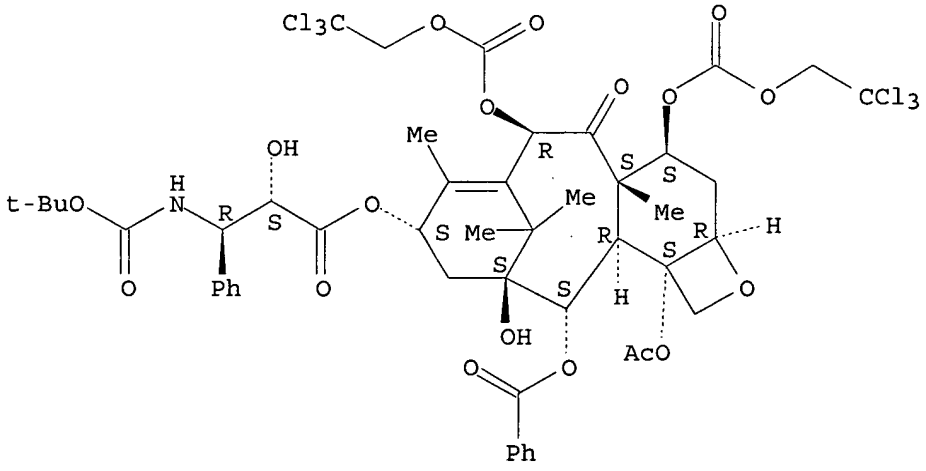
AB The title compds. [I; R = H, OAc; R1 = (2'R,3'S)-COCH(OH)CHPhNHBz; R2 = H] were prepared as antitumor agents (no data). I (R = R2 = CO2CH2CCl3, R1 = COCH:CHPh) (preparation given) was added to an MeCN solution of Me3CO2CNClNa (treated with AgNO3) and OsO4 and the mixture stirred 68 h in the dark with addnl. reagent addition to give I [R1 = COCH(OH)CHPhNHCO2CMe3, R, R2 as above] which was stirred at 0° in MeCN with Me3SiI to give I [R1 = COCH(OH)CHPhNH2, R, R2 as above]. The latter were stirred in pyridine with BzCl to give I [R1 = COCH(OH)CHPhNHBz, R, R2 as above] which was stirred 2 h in HOAc containing Zn to give I [R = R2 = H, R1 = COCH(OH)CHPhNHBz].

IT **114977-25-2P**
RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in preparation of antitumor agents)

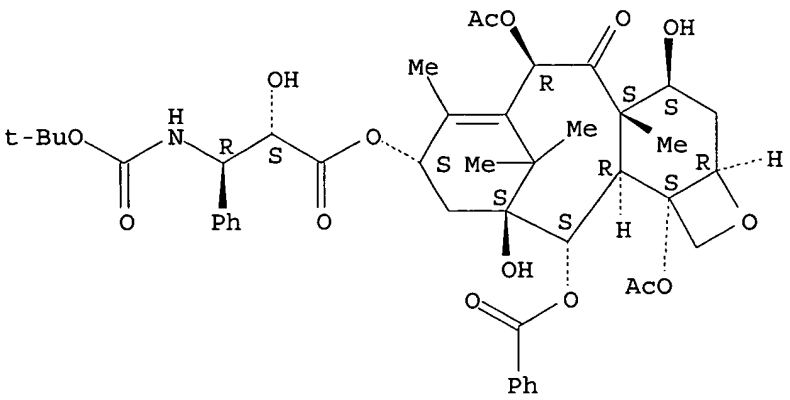
RN 114977-25-2 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 52 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:422762 CAPLUS



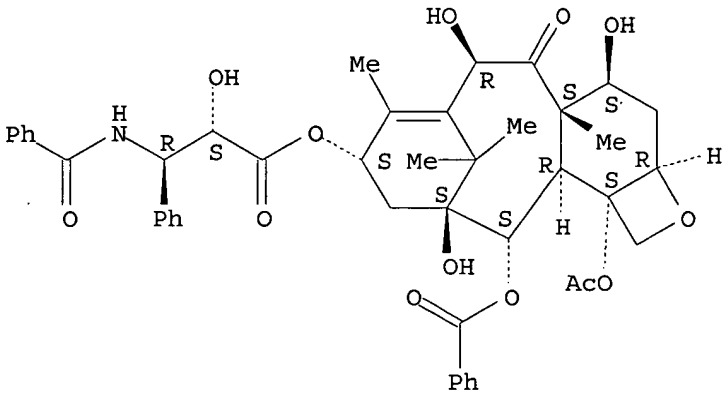
L51 ANSWER 51 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:422763 CAPLUS
DOCUMENT NUMBER: 109:22763
TITLE: Preparation of taxol and of 10-desacetyl-10-taxol as antitumor agents
INVENTOR(S): Colin, Michel; Guenard, Daniel; Gueritte-Voegelein, Francoise; Potier, Pierre
PATENT ASSIGNEE(S): Rhone-Poulenc Sante, Fr.
SOURCE: Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 253739	A1	19880120	EP 1987-401669		19870716
EP 253739	B1	19891011			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
FR 2601676	A1	19880122	FR 1986-10401		19860717
FR 2601676	B1	19880923			
US 4857653	A	19890815	US 1987-73154		19870714
AU 8775678	A1	19880121	AU 1987-75678		19870715
AU 591310	B2	19891130			
ZA 8705180	A	19880330	ZA 1987-5180		19870715
JP 63030478	A2	19880209	JP 1987-176070		19870716
JP 06004607	B4	19940119			
AT 47137	E	19891015	AT 1987-401669		19870716
CA 1278303	A1	19901227	CA 1987-542297		19870716
PRIORITY APPLN. INFO.:			FR 1986-10401	A	19860717
			EP 1987-401669	A	19870716

OTHER SOURCE(S): MARPAT 109:22763
GI

tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

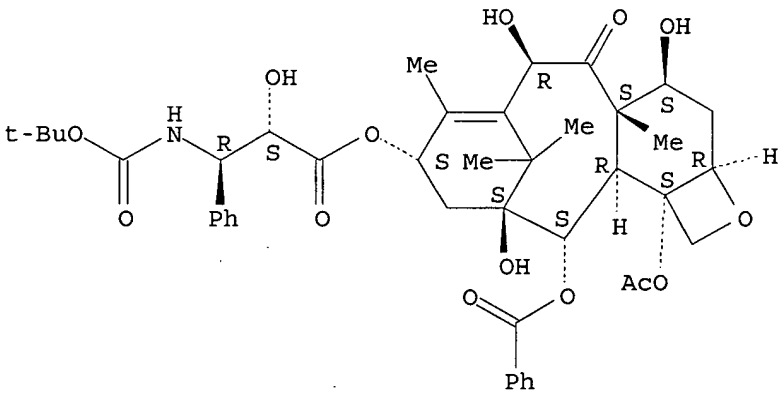


IT **114977-29-6P 125354-17-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as taxol analog)

RN 114977-29-6 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

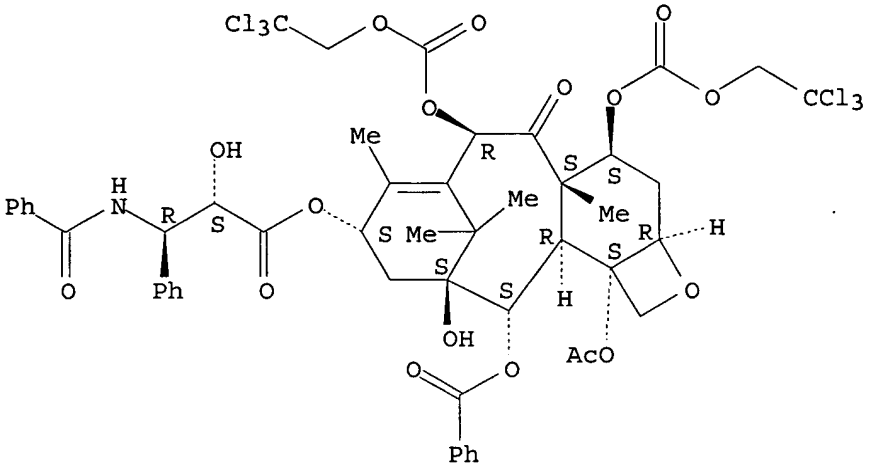
Absolute stereochemistry.



RN 125354-17-8 CAPLUS

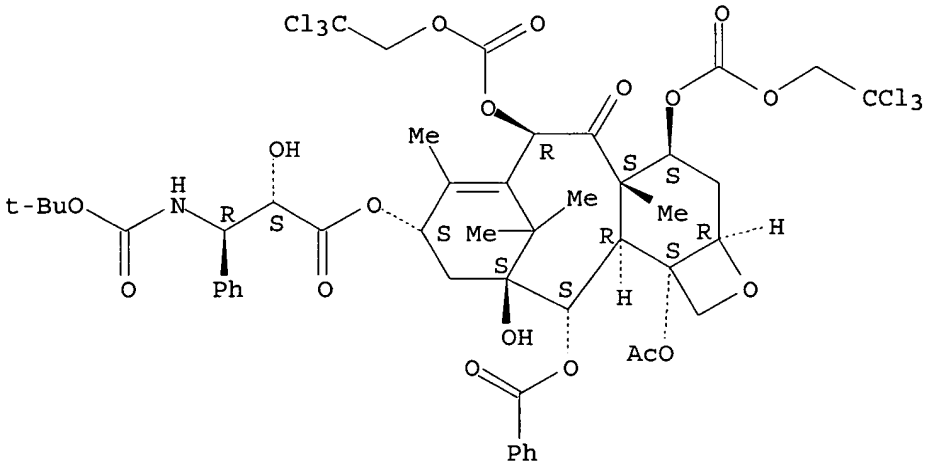
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

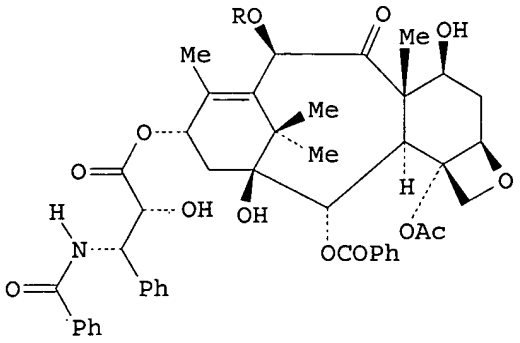


IT **114977-25-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and detrichloroethoxycarbonylation or de-tert-butyloxycarbonylation of)
RN 114977-25-2 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

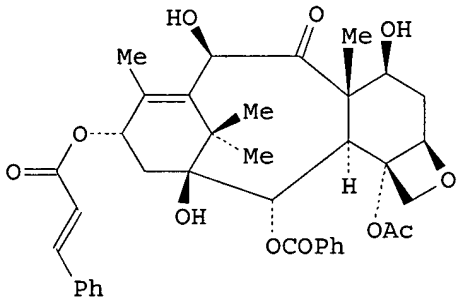
Absolute stereochemistry.



IT **125354-13-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as deacetyltaxol analog)
RN 125354-13-4 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-



I



II

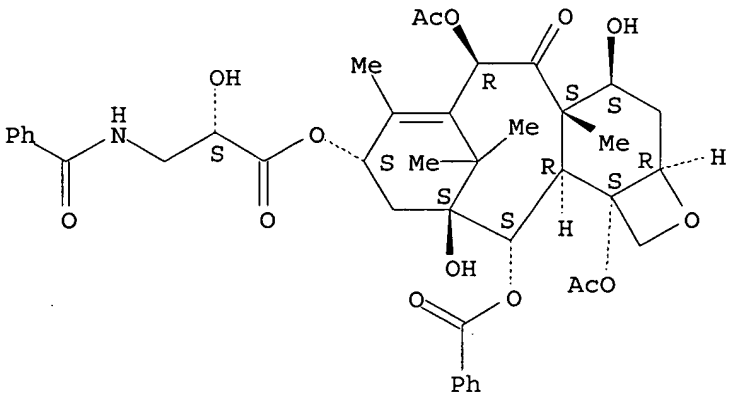
AB Taxol (I; R = Ac) 10-deacetyltaxol (I; R = H) and their side chain analogs were obtained via a Sharpless oxyamination reaction on 13-cinnamoylbaccatin III (II). Asym. induction was studied using different bridgehead amines as chiral ligands. This procedure constitutes an alternative route to taxol derivs. for biol. studies.

IT **125354-12-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and detrichloroethoxycarbonylation of)

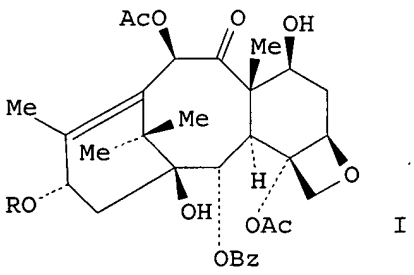
RN 125354-12-3 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(.alpha.S*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 50 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:119169 CAPLUS
DOCUMENT NUMBER: 112:119169
TITLE: Application of the vicinal hydroxyamination reaction with asymmetric induction to the hemisynthesis of taxol and analogs
AUTHOR(S): Mangatal, L.; Adeline, M. T.; Guenard, D.; Gueritte-Voegelein, F.; Potier, P.
CORPORATE SOURCE: Inst. Chim. Subst. Nat., CNRS, Gif-sur-Yvette, 91198, Fr.
SOURCE: Tetrahedron (1989), 45(13), 4177-90
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:119169
GI



I

AB Taxol (I, R = H) a potent inhibitor of cell replication, enhances the assembly of tubulin into stable microtubules and promotes the formation of microtubule bundles in cells. In addition to its unique mechanism of action, taxol exhibits unusual promise as an antitumor agent, but its application in cancer chemotherapy is hampered by its limited availability. In order to better define the structure-activity profile of taxol or the design of more accessible drugs and to provide insight into the chemical features of the taxol-microtubule interaction, taxol analogs I [R = (R)-, (S)-HOCHMeCO, HOCH(CH2Ph)CO, BzNHCH2CH(OH)CO] were synthesized from baccatin III through esterification at the hindered 13-hydroxyl. Although less biol. active than taxol, analogs I [R = (R)-, and (S)-PhCH2CH(OH)CO, R-BzNHCH2CH(OH)CO] promote the polymerization of tubulin and are cytotoxic; I [R = PhCH2CH(OH)CO] were most effective. Interestingly, tubulin polymerization was sensitive to the C-2' configuration only when the amide substituent was present in the side chain. This observation suggests that the 3'-amide substituent plays an important role in preorganizing the taxol side chain to bind to microtubules.

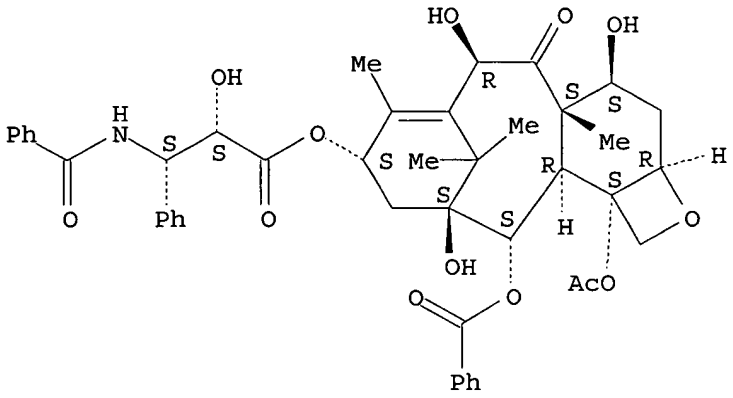
IT **131896-67-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and tubulin polymerization by)

RN 131896-67-8 CAPLUS

CN Propanoic acid, 3-(benzoylamino)-2-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(S*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

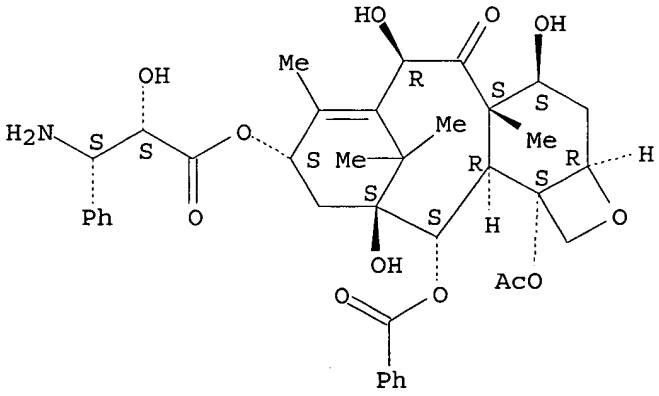
Absolute stereochemistry.

Absolute stereochemistry.

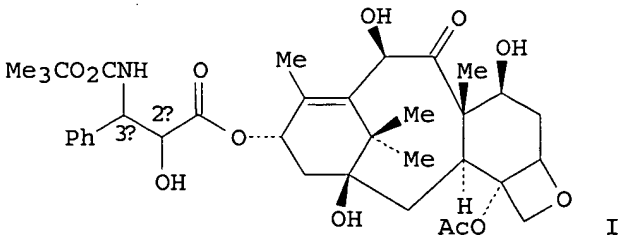


RN 133577-37-4 CAPLUS
CN Benzenepropanoic acid, β-amino-α-hydroxy-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L51 ANSWER 49 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:122749 CAPLUS
DOCUMENT NUMBER: 114:122749
TITLE: Biologically active taxol analogs with deleted A-ring side chain substituents and variable C-2' configurations
AUTHOR(S): Swindell, Charles S.; Krauss, Nancy E.; Horwitz, Susan B.; Ringel, Israel
CORPORATE SOURCE: Dep. Chem., Bryn Mawr Coll., Bryn Mawr, PA, 19010, USA
SOURCE: Journal of Medicinal Chemistry (1991), 34(3), 1176-84
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

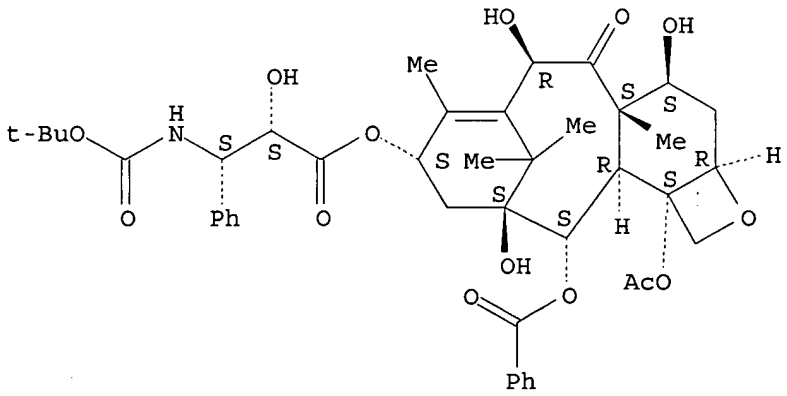
AB A variety of synthetic analogs of taxol, a naturally occurring antitumor diterpene, were examined for their potency to inhibit microtubule disassembly. For some of the compds., the in vitro cytotoxic properties showed a good correlation with the tubulin assay. This structure-activity relationship study confirms that inhibition of microtubule disassembly is quite sensitive to the configuration at C-2' and C-3'. A correlation between the conformation of the side chain at C-13 and the activity is suggested. Of all the compds. examined, one of the most potent in inhibiting microtubule disassembly and in inhibiting murine P388 leukemic cells, N-debenzoyl-N-tert-(butoxycarbonyl)-10-deacetyltaxol, named taxotere [(2'R,3'S)-I], was selected for evaluation as a potential anticancer agent.

IT **133577-33-0P 133577-35-2P 133577-37-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as inhibitor of microtubule disassembly)

RN 133577-33-0 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 133577-35-2 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

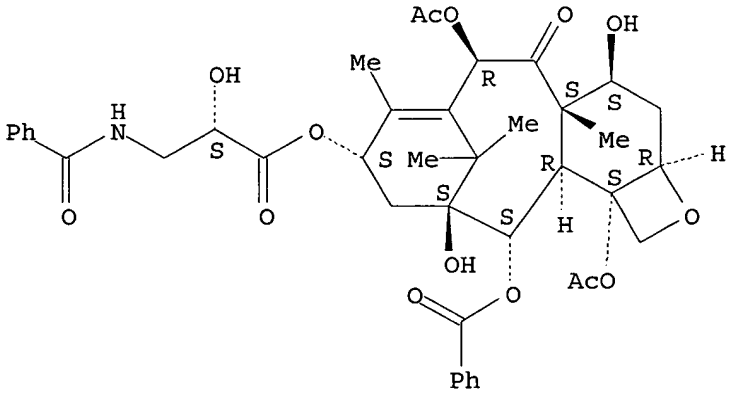
activity. The importance of the side chain was shown by the much lower activity as compared to taxol of analogs lacking all or part of the side chain. The effect of stereochem. at the C-2' position on fungitoxicity towards oomycetes was similar to that reported previously on mammalian microtubule assembly.

IT **131896-67-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(fungicidal activity of, structure in relation to)

RN 131896-67-8 CAPLUS

CN Propanoic acid, 3-(benzoylamino)-2-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(S*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 48 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:247557 CAPLUS

DOCUMENT NUMBER: 114:247557

TITLE: Relationships between the structure of taxol analogs and their antimitotic activity

AUTHOR(S): Gueritte-Voegelein, Francoise; Guenard, Daniel; Lavelle, Francois; Le Goff, Marie Therese; Mangatal, Lydie; Potier, Pierre

CORPORATE SOURCE: Inst. Chim. Subst. Nat., Gif-sur-Yvette, 91198, Fr.

SOURCE: Journal of Medicinal Chemistry (1991), 34(3), 992-8
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

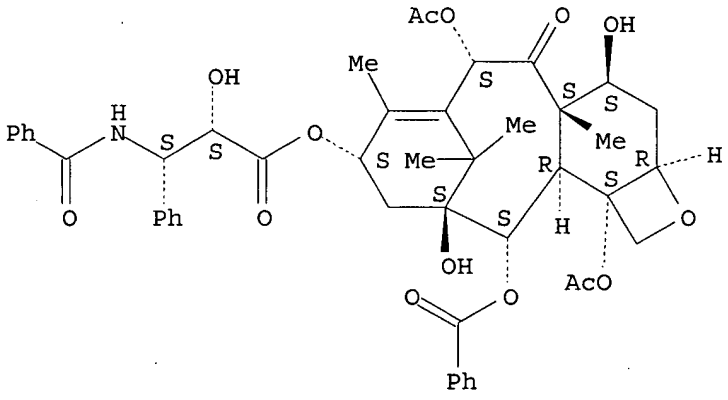
AB Low-toxicity, antitumor compound NSC-LSC1 I, a taxol analog, is manufactured with
a callus culture developed from albumens of Taxus, especially Taxus brevifolia. In vitro antitumor activity of I was shown by its IC50 against the mouse leukemic cells P388 and human squamous carcinoma cells KB, 3.3 and 19 ng/mL, resp.

IT **147557-12-8P**
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, with callus culture of Taxus brevifolia, as antitumor agent)

RN 147557-12-8 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6α,9α(αS*,βS*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

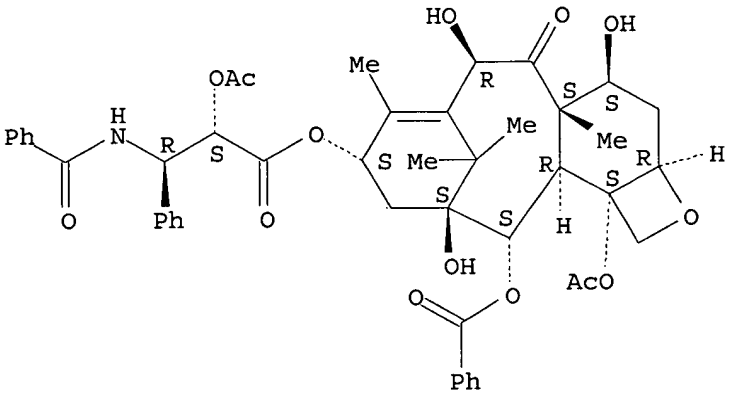


L51 ANSWER 47 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:55951 CAPLUS
DOCUMENT NUMBER: 118:55951
TITLE: Antifungal properties of taxol and various analogs
AUTHOR(S): Young, D. H.; Michelotti, E. L.; Swindell, C. S.; Krauss, N. E.
CORPORATE SOURCE: Res. Lab., Rohm and Haas Co., Spring House, PA, 19477, USA
SOURCE: Experientia (1992), 48(9), 882-5
CODEN: EXPEAM; ISSN: 0014-4754
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The antimitotic agent taxol was tested for toxicity towards fungi from different taxonomic groups and found to be particularly active against oomycete fungi. In terminating zoospore cysts of the oomycete Phytophthora capsici the mechanism of action of taxol was shown to involve inhibition of mitosis, presumably resulting from an effect on microtubules. Various taxol analogs with deleted A-ring C-13 side chain substituents were tested for toxicity towards P. capsici and Aphanomyces cochlioides to provide insight into structural features required for

RN 151509-29-4 CAPLUS
CN Benzenepropanoic acid, α-(acetyloxy)-β-(benzoylamino)-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

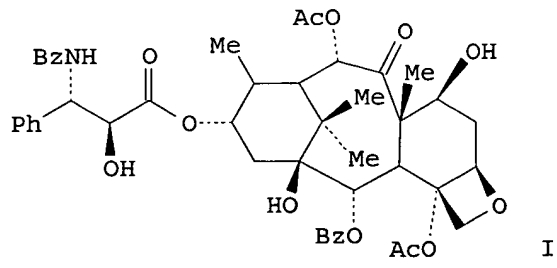
Absolute stereochemistry.



L51 ANSWER 46 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:232375 CAPLUS
DOCUMENT NUMBER: 118:232375
TITLE: Antitumor compound NSC-LSC1 and its manufacture with callus culture of Taxus brevifolia
INVENTOR(S): Saito, Koji; Ohashi, Hiroaki; Tahara, Makoto; Sakamoto, Tetsuo; Hibi, Masaaki
PATENT ASSIGNEE(S): Nippon Steel Corp., Japan
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9302067 A1		19930204	WO 1992-JP917	19920717
W: CA, JP, KR, US				
RW: AT, BE, CH, DE, FR, GB, IT, SE				
PRIORITY APPLN. INFO.:			JP 1991-176902	19910717

GI



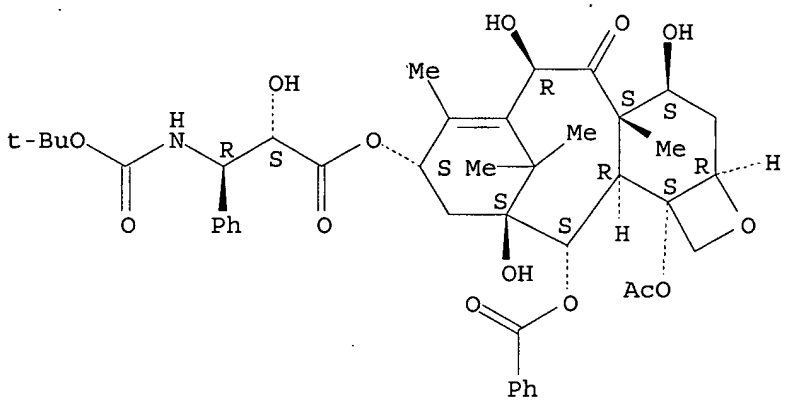
I

= OH, R2 = NHCO2CMe3), possess a different conformation with no hydrophobic interactions between the side chain and the taxan skeleton.

IT **114977-29-6 133577-33-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(conformation determined by NMR and mol. modeling)

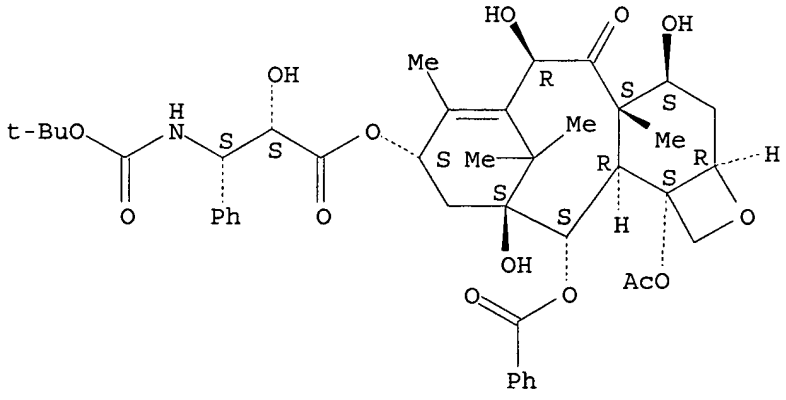
RN 114977-29-6 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

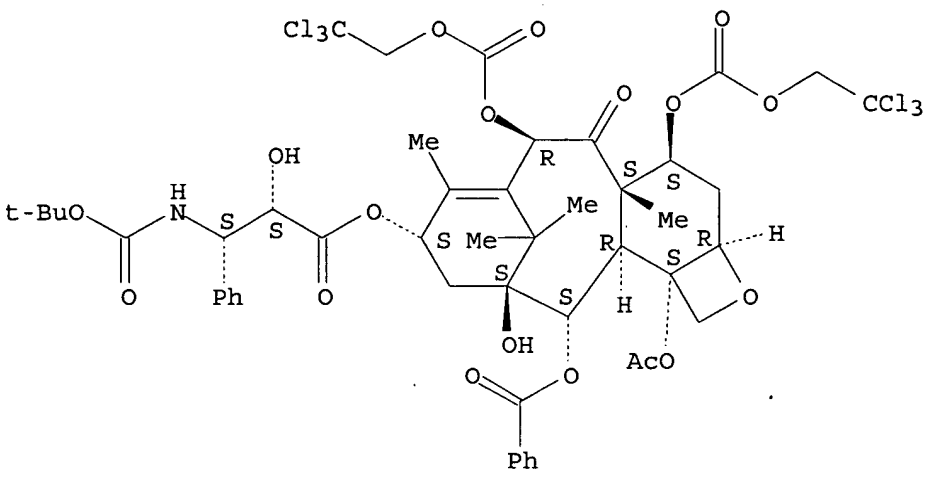


RN 133577-33-0 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

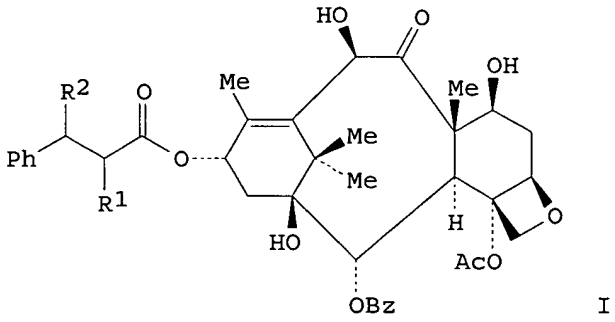
Absolute stereochemistry.



IT **151509-29-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation determined by NMR and mol. modeling)



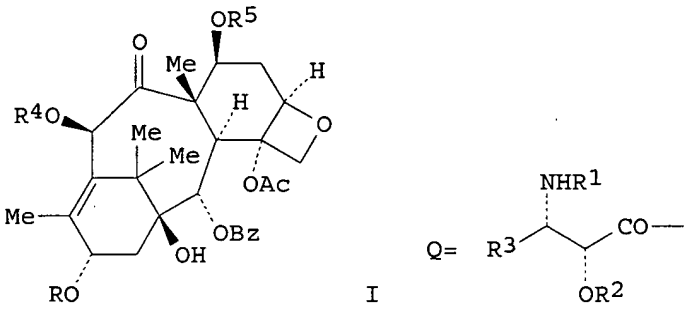
L51 ANSWER 45 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:8769 CAPLUS
DOCUMENT NUMBER: 120:8769
TITLE: Conformation of Taxotere and analogs determined by NMR spectroscopy and molecular modeling studies
AUTHOR(S): Dubois, Joelle; Guenard, Daniel; Gueritte-Voegelein, Francoise; Guedira, Nourredine; Potier, Pierre; Gillet, Brigitte; Beloeil, Jean Claude
CORPORATE SOURCE: Inst. Chim. Subst. Nat., CNRS, Gif-sur-Yvette, 91198, Fr.
SOURCE: Tetrahedron (1993), 49(30), 6533-44
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The conformation of Taxotere (2'R,3'S)-I (R1 = OH, R2 = NHCO2CMe3) and its analogs, (2'R)-I (R1 = OH, R2 = H), (3'R)-I (R1 = H, R2 = NHCO2CMe3), (2'S,3'R)-I (R1 = O2CMe, R2 = NHBz), etc., was determined by NMR spectroscopy and mol. modeling. The most active 2'R,3'S compds. possess a conformation in which the benzoate group at C-2 holds the side chain in a defined position due to hydrophobic interactions between this group and the N-amido or N-carbonyloxy group at C-3'. On the other hand, the 2'S,3'R isomers which display low in vivo biol. activity, such as (2'S,3'R)-I (R1

FI 106959 B1 20010515
PRIORITY APPLN. INFO.: FR 1992-1379 A 19920207
WO 1993-FR110 A 19930204
OTHER SOURCE(S): CASREACT 120:30979; MARPAT 120:30979
GI



I

AB Title compds. (I; R = aminohydroxypropionyl group Q; R1 = Bz, COCMe3; R2 = H; R3 = aryl; R4 = H or Ac; R5 = H) were prepared by condensation of QOH (R2 = hydroxy-protective group) with I (R = H, R4 = Ac or hydroxy-protective group, R5 = hydroxy-protective group). Thus, I (R4 = R5 = CO2CH2CF3) (II; R = H) was stirred 72 h at -10° with (2R,3S)-PhCH(NHCO2CMe3)CH[OCH(OEt)Me]CO2H in PhMe containing DCC and 4-pyrrolidinopyridine to give 97% II [R = COCH(OH)CHPhNCO2CMe3] with 12.7% epimerization at C-2 of the acid moiety.

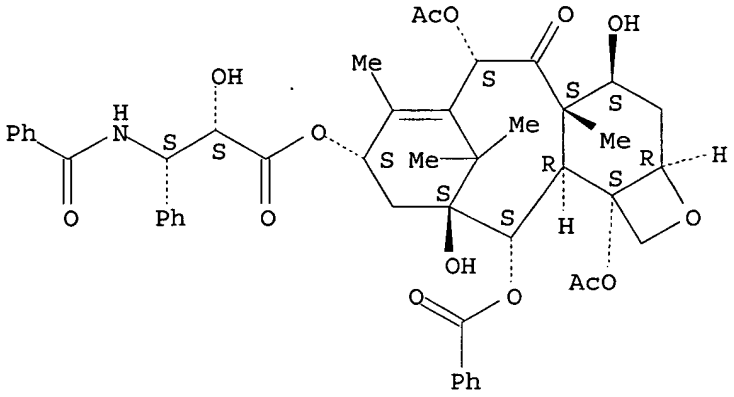
IT **151636-78-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 151636-78-1 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.



L51 ANSWER 44 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:30979 CAPLUS
DOCUMENT NUMBER: 120:30979
TITLE: Method for preparing taxane derivatives
INVENTOR(S): Fouque, Elie; Mas, Jean Manuel
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer SA, Fr.
SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9316059	A1	19930819	WO 1993-FR110	19930204
W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, PL, RU, SK, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2687150	A1	19930813	FR 1992-1379	19920207
FR 2687150	B1	19950428		
AU 9335048	A1	19930903	AU 1993-35048	19930204
AU 686095	B2	19980205		
EP 625147	A1	19941123	EP 1993-904150	19930204
EP 625147	B1	19960828		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07503472	T2	19950413	JP 1993-513563	19930204
JP 3295879	B2	20020624		
HU 68773	A2	19950728	HU 1994-2289	19930204
HU 212577	B	19960829		
AT 141920	E	19960915	AT 1993-904150	19930204
ES 2090970	T3	19961016	ES 1993-904150	19930204
RU 2103266	C1	19980127	RU 1994-40356	19930204
CZ 283377	B6	19980415	CZ 1994-1870	19930204
PL 175106	B1	19981130	PL 1993-304721	19930204
SK 280012	B6	19990712	SK 1994-930	19930204
CA 2126462	C	20020709	CA 1993-2126462	19930204
ZA 9300823	A	19930916	ZA 1993-823	19930205
US 6596880	B1	20030722	US 1994-256736	19940802
NO 9402895	A	19940804	NO 1994-2895	19940804
NO 305863	B1	19990809		
FI 9403643	A	19940805	FI 1994-3643	19940805

Correction of: 118:232375

TITLE: Antitumor compound NSC-LSC1 and its manufacture with callus culture of Taxus brevifolia

INVENTOR(S): Saito, Koji; Ohashi, Hiroaki; Tahara, Makoto; Sakamoto, Tetsuo

PATENT ASSIGNEE(S): Nippon Steel Corp., Japan

SOURCE: PCT Int. Appl., 1 p.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

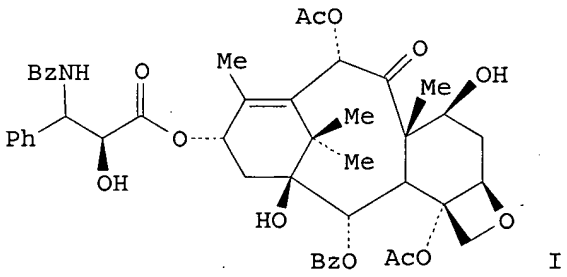
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9302067	A1	19930204	WO 1992-JP917		19920717
W: CA, JP, KR, US					
RW: AT, BE, CH, DE, FR, GB, IT, SE					
CA 2092705	AA	19930118	CA 1992-2092705		19920717
CA 2092705	C	19951107			
EP 555485	A1	19930818	EP 1992-915865		19920717
R: AT, BE, CH, DE, FR, GB, IT, LI, SE					
PRIORITY APPLN. INFO.:			JP 1991-176902	A	19910717
			WO 1992-JP917	W	19920717

GI



I

AB Low-toxicity, antitumor compound NSC-LSC1 (I), a taxol analog, is manufactured with a callus culture developed from albumens of Taxus, especially Taxus brevifolia. In vitro antitumor activity of I was shown by its IC50 of 3.3 and 19 ng/mL against P388 mouse leukemia cells and KB human squamous carcinoma cells, resp.

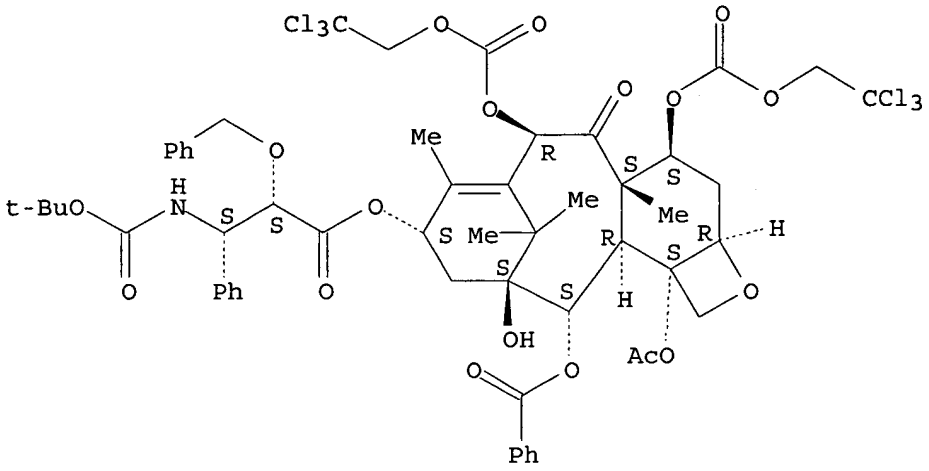
IT **147557-12-8P**
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, with callus culture of Taxus brevifolia, as antitumor agent)

RN 147557-12-8 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6α,9α(αS*,βS*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

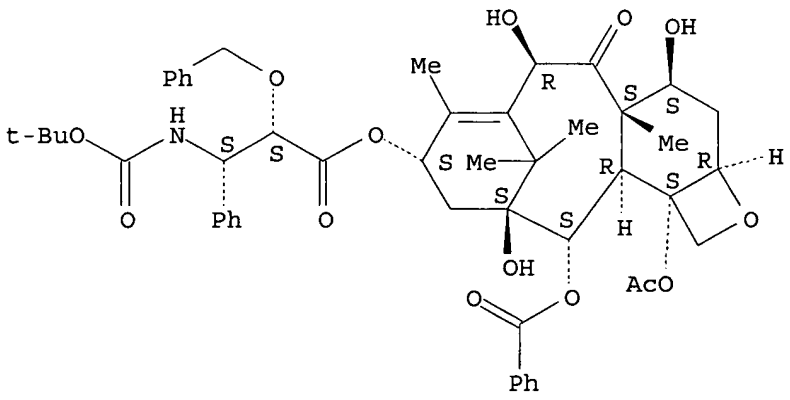
methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

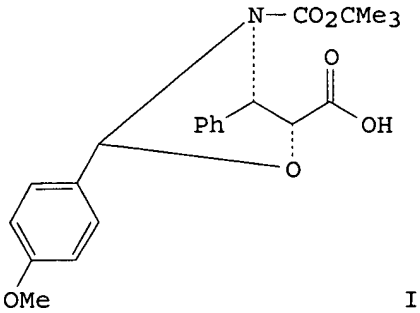


IT **155487-38-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of, taxotere from)
RN 155487-38-0 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-(phenylmethoxy)-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

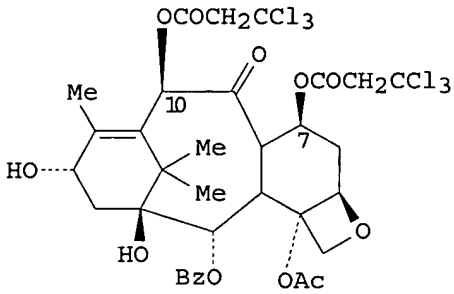
Absolute stereochemistry.



L51 ANSWER 43 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:242670 CAPLUS
Correction of: 1993:232375
DOCUMENT NUMBER: 120:242670



I



III

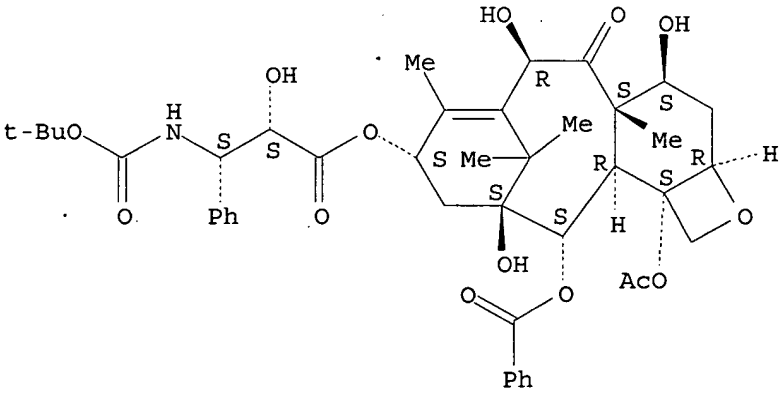
AB A high-yield synthesis of the p-methoxybenzylidene-protected docetaxel (Taxotere) side chain I, a useful derivative for efficient, epimerization-free esterification of the 7,10-bis[(trichloroethoxy)carbonyl] derivative II of 10-desacetylbaccatin III for the preparation of docetaxel, has been effected. The C-4 and C-5 stereocenters of the 1,3-oxazolidine are generated with complete (≥99%) stereocontrol whereas that at C-2 is produced with 96% selectivity.

IT **133577-33-0P**, 2'-epi-Taxotere
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in synthesis of taxotere)

RN 133577-33-0 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **155487-37-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and de(trichloroethoxy)carbonylation of, in synthesis of taxotere)

RN 155487-37-9 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-(phenylmethoxy)-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-

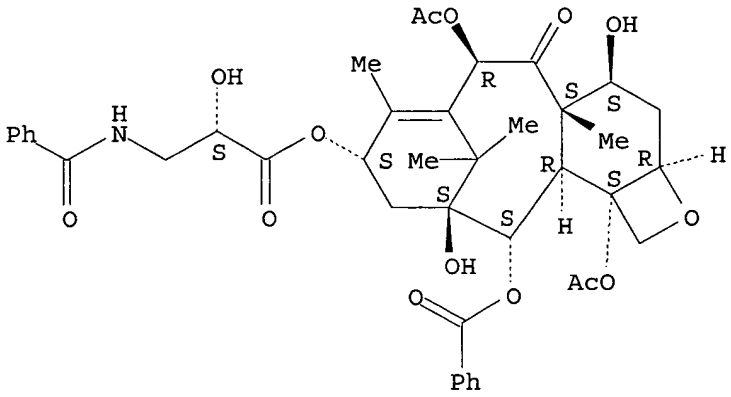
the same precision as had been possible for taxol, but the conformational possibilities could be significantly limited by the data. Analogs I [(2'R), R = Ac, R1 = H, R2 = NHCO2Bz; (2'R), R = Ac, R1 = Ph, R2 = H; (2'S), R = Ac, R1 = Ph, R2 = H] , but not (2'S)-I (R = Ac, R1 = H, R2 = NHCO2Bz), can mimic the dominant conformation of taxol in chloroform, but no logical relationship between biol. activity and aqueous solution conformation could be detected.

IT **131896-67-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 131896-67-8 CAPLUS

CN Propanoic acid, 3-(benzoylamino)-2-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(S*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 42 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:435897 CAPLUS

DOCUMENT NUMBER: 121:35897

TITLE: Highly Stereocontrolled and Efficient Preparation of the Protected, Esterification-Ready Docetaxel (Taxotere) Side Chain

AUTHOR(S): Kanazawa, Alice M.; Denis, Jean-Noel; Greene, Andrew E.

CORPORATE SOURCE: Universite Joseph Fourier de Grenoble, Grenoble, 38041, Fr.

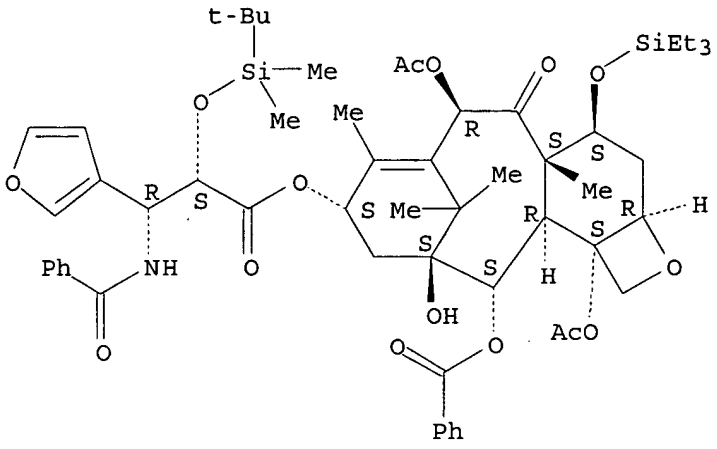
SOURCE: Journal of Organic Chemistry (1994), 59(6), 1238-40
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

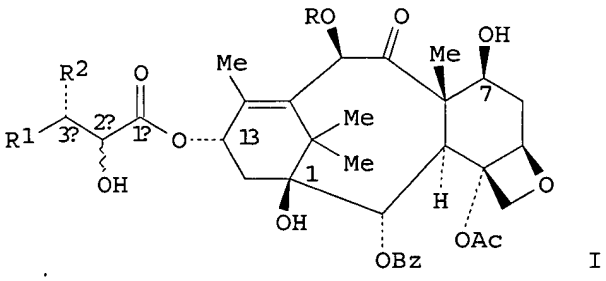
LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:35897

GI



L51 ANSWER 41 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:483667 CAPLUS
DOCUMENT NUMBER: 121:83667
TITLE: NMR and molecular modeling study of active and inactive taxol analogs in aqueous and nonaqueous solution
AUTHOR(S): Williams, Howard J.; Scott, A. Ian; Dieden, Reiner A.; Swindell, Charles S.; Chirlian, Lisa E.; Francl, Michelle M.; Heerding, Julia M.; Krauss, Nancy E.
CORPORATE SOURCE: Cent. Biol. NMR, Texas A and M Univ., College Station, TX, 77843-3255, USA
SOURCE: Canadian Journal of Chemistry (1994), 72(1), 252-60
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

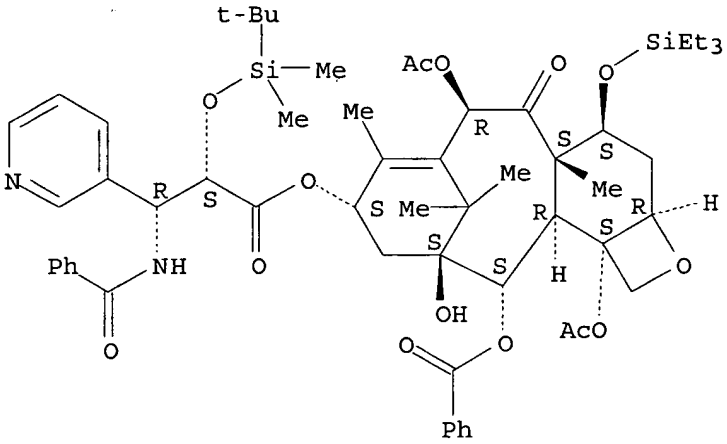
AB The conformations of the biol. active taxol analogs Taxotere [(2'R)-I; R = H, R1 = Ph, R2 = NHCO2CMe3], (2'R)-I (R = Ac, R1 = H, R2 = NHCO2Bz), (2'R)-I (R = Ac, R1 = Ph, R2 = H), and (2'S)-I (R = Ac, R1 = Ph, R2 = H), and the biol. inactive analog (2'S)-I (R = Ac, R1 = H, R2 = NHCO2Bz) were evaluated in CDCl3 and DMSO-water solution using 1H NMR coupling constant and NOESY data and mol. modeling. The solution structures of Taxotere were very similar to those detected previously for taxol [(2'R)-I; R = Ac, R1 = Ph, R2 = NHCO2Bz]. The A-ring side chain conformations of analogs I (R = Ac, R1 = H, R2 = NHCO2Bz; R = Ac, R1 = Ph, R2 = H) could not be defined with

(R1 = 2-furyl) proved to be more active than the parent, taxol.

IT **158412-29-4P 158412-30-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of taxol analogs)

RN 158412-29-4 CAPLUS
CN 3-Pyridinepropanoic acid, β-(benzoylamino)-α-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

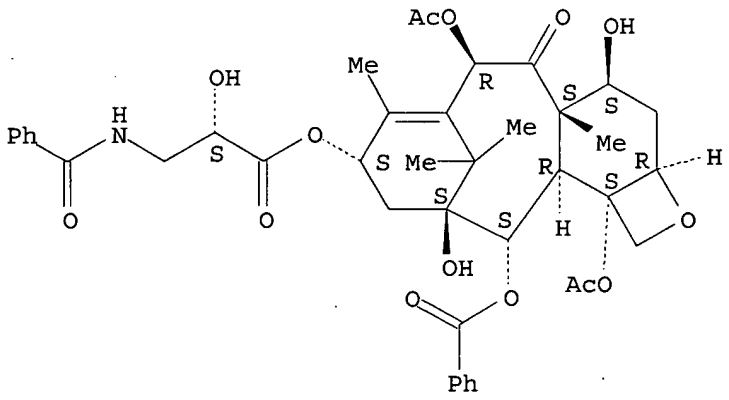
Absolute stereochemistry.



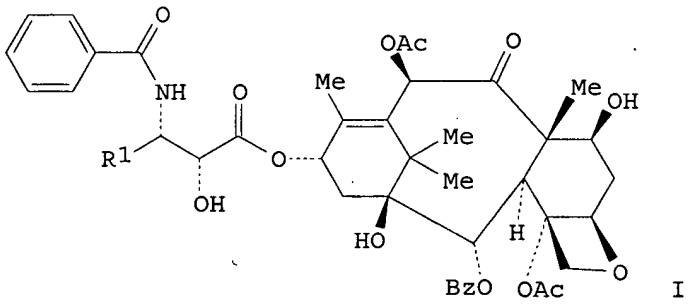
RN 158412-30-7 CAPLUS
CN 3-Furanpropanoic acid, β-(benzoylamino)-α-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

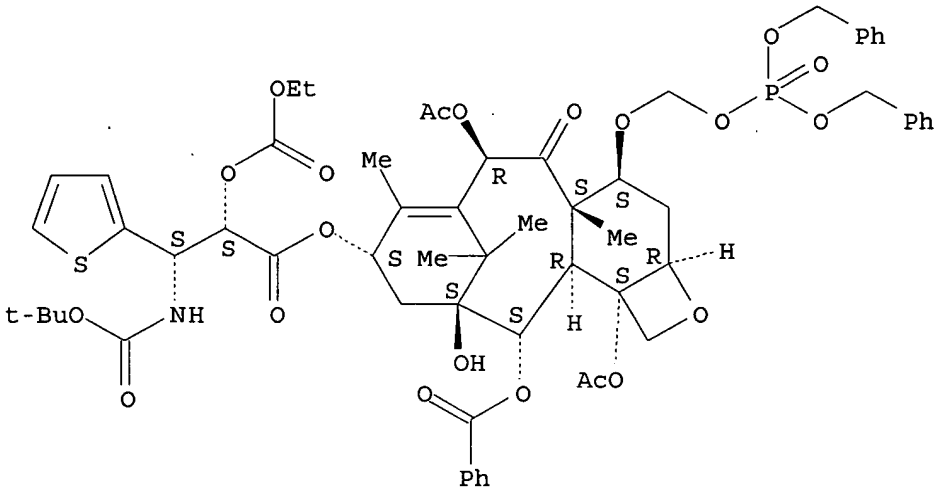


L51 ANSWER 40 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:656068 CAPLUS
DOCUMENT NUMBER: 121:256068
TITLE: Heteroaromatic taxol analogs: the chemistry and biological activities of 3'-furyl and 3'-pyridyl substituted taxanes
AUTHOR(S): Georg, Gunda I.; Harriman, Geraldine C. B.; Hepperle, Michael; Himes, Richard H.
CORPORATE SOURCE: Dep. Medicinal Chem., Univ. Kansas, Lawrence, KS, 66045, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(11), 1381-4
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A series of novel heterocyclic taxol analogs I (R1 = 2-, 3-, 4-pyridyl, 2-, 3-furyl) has been synthesized utilizing 2-azetidinones derived from the ester enolate-imine cyclocondensation. 2-Azetidinones possessing stereochem. complementary to that of taxol's phenylisoserine side chain were synthesized in fair to high enantiomeric purity utilizing the chiral glycolate derived from Oppolzer's chiral auxiliary and the appropriate N-trimethylsilylaldimines. I were evaluated in the microtubule assembly assay as well as tested for cytotoxicity against B16 melanoma cells. I

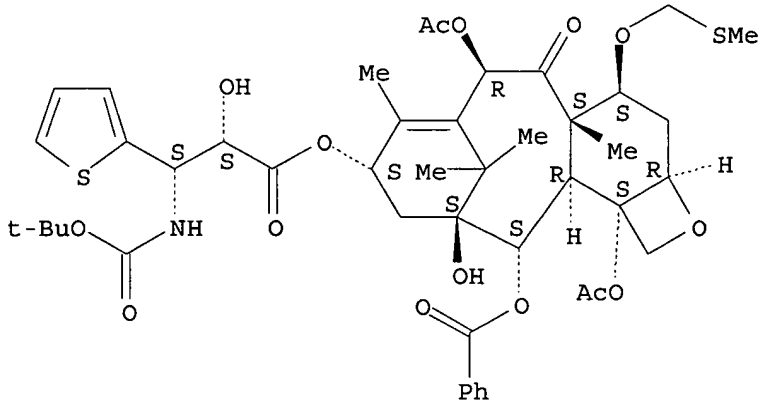


L51 ANSWER 39 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:209891 CAPLUS
DOCUMENT NUMBER: 122:45673
TITLE: Relationship between the structure of taxol and other taxanes on induction of tumor necrosis factor-α gene expression and cytotoxicity
AUTHOR(S): Burkhart, Catherine A.; Berman, Joan W.; Swindell, Charles S.; Horwitz, Susan Band
CORPORATE SOURCE: Dep. Mol. Pharmacol., Albert Einstein Coll. Med., Bronx, NY, 10461, USA
SOURCE: Cancer Research (1994), 54(22), 5779-82
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Taxol is an antitumor drug with cytotoxic properties that correlate with its microtubule-stabilizing activities. It has been reported that taxol parallels lipopolysaccharide in its effects on the induction of tumor necrosis factor-α (TNF-α) gene expression in macrophages. Structure-activity studies using taxol and related taxanes have been done to determine the relationship between the effects of taxol on TNF-α gene expression and its cytotoxic and microtubule-stabilizing activities. Using Northern blot anal., it was found that changes in the structure of taxol that did not alter cytotoxicity did prevent the induction of TNF-α gene expression. The data presented in this paper demonstrate that the effects of taxol on TNF-α gene expression are distinct from its known cytotoxic properties.

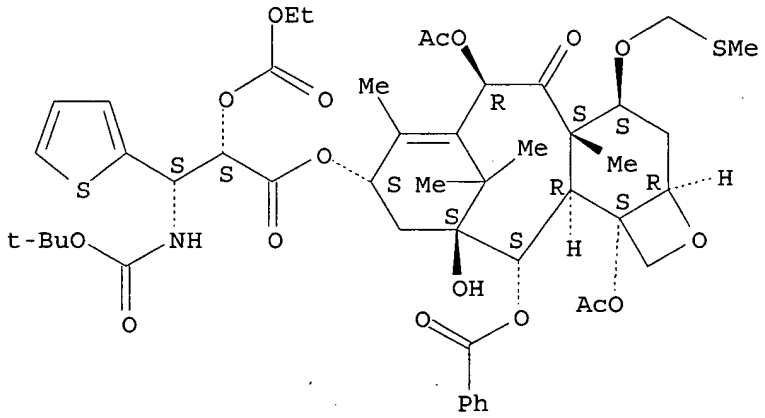
IT **131896-67-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(relationship between structure of taxol and other taxanes on induction of tumor necrosis factor-α gene expression and cytotoxicity)

RN 131896-67-8 CAPLUS
CN Propanoic acid, 3-(benzoylamino)-2-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(S*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)



RN 162871-22-9 CAPLUS
CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(ethoxycarbonyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-4-[(methylthio)methoxy]-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 162871-23-0 CAPLUS
CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(ethoxycarbonyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-4-[[[bis(phenylmethoxy)phosphinyl]oxy]methoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

OTHER SOURCE(S): MARPAT 122:291219

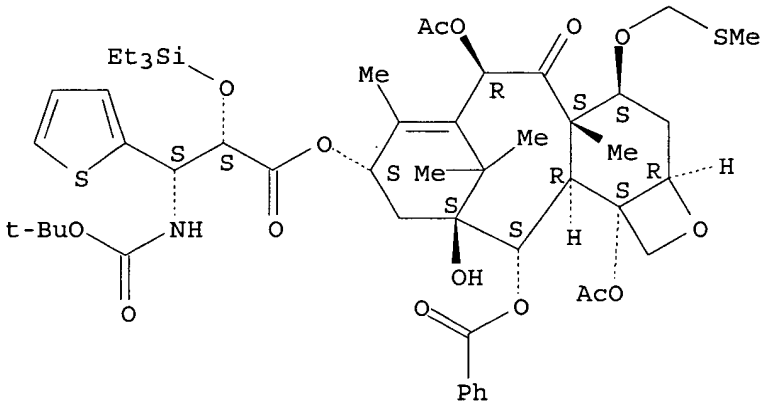
AB Taxane derivs. T-[OCH2(OCH2)mOP(O)(OH)2]n [T = taxane substituted at C-13 by 3-amino-2-hydroxypropanoyloxy; m = 0-6; n = 1-3] were prepared from paclitaxel or baccatin III via T'-[OCH2(OCH2)mSMe]n [T' = protected T] for use as antitumor agents. Thus, paclitaxel was converted to its 7-O-methylthiomethyl derivative, treated with dibenzyl phosphate, followed by hydrogenolysis to give 7-O-phosphonooxymethylpaclitaxel. This compound had an IC50 against HCT-116 human carcinoma of 0.0158 μM. Some of the methylthiomethyl derivs. also have antitumor activity.

IT **162871-20-7P 162871-21-8P 162871-22-9P**
162871-23-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phosphonooxymethyl or methylthiomethyl ethers of taxane derivs. as antitumor agents.)

RN 162871-20-7 CAPLUS

CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-4-[(methylthio)methoxy]-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 162871-21-8 CAPLUS

CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-4-[(methylthio)methoxy]-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L51 ANSWER 38 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:526804 CAPLUS
DOCUMENT NUMBER: 122:291219
TITLE: Phosphonooxymethyl or methylthiomethyl ethers of taxane derivatives as antitumor agents.
INVENTOR(S): Golik, Jerzy; Kadow, John F.; Kaplan, Murray A.; Li, Wen-Sen; Perrone, Robert K.; Thottathil, John K.; Vyas, Dolatrai; Wittman, Mark D.; Wong, Henry; Wright, John J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: Eur. Pat. Appl., 124 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

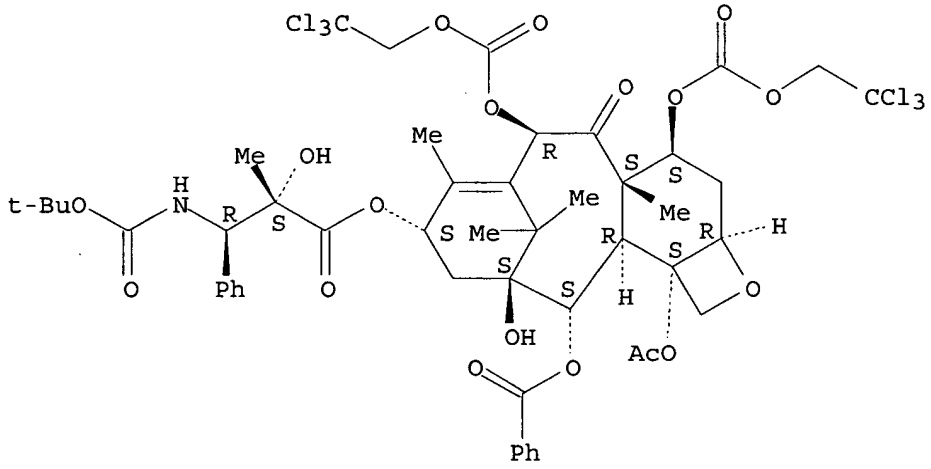
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 639577	A1	19950222	EP 1994-112803	19940816
EP 639577	B1	20020515		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
IL 122990	A1	20020523	IL 1993-122990	19931223
IL 148029	A1	20050517	IL 1993-148029	19931223
CA 2129288	AA	19950218	CA 1994-2129288	19940802
CA 2129288	C	20000516		
HU 67742	A2	19950428	HU 1994-2342	19940812
JP 07149779	A2	19950613	JP 1994-250219	19940812
JP 3062986	B2	20000712		
FI 9403749	A	19950218	FI 1994-3749	19940815
FI 113271	B1	20040331		
NO 9403002	A	19950220	NO 1994-3002	19940815
NO 309093	B1	20001211		
AU 9470267	A1	19950302	AU 1994-70267	19940815
AU 694941	B2	19980806		
CN 1111637	A	19951115	CN 1994-109468	19940815
CN 1051315	B	20000412		
RU 2128661	C1	19990410	RU 1994-29662	19940815
ZA 9406180	A	19950216	ZA 1994-6180	19940816
PL 179636	B1	20001031	PL 1994-304649	19940816
AT 217629	E	20020615	AT 1994-112803	19940816
PT 639577	T	20021031	PT 1994-112803	19940816
ES 2176212	T3	20021201	ES 1994-112803	19940816
US 5646176	A	19970708	US 1995-445360	19950519
US 2001023255	A1	20010920	US 1997-870794	19970606
US 6455575	B2	20020924		
AU 9891356	A1	19990114	AU 1998-91356	19981106
AU 706511	B2	19990617		
CN 1237580	A	19991208	CN 1999-105343	19990429
CN 1100771	B	20030205		

PRIORITY APPLN. INFO.:

US 1993-108015	A	19930817
US 1993-154840	A	19931124
US 1994-245119	A	19940517
US 1992-996455	B2	19921224
IL 1993-108161	A3	19931223
IL 1993-122990	A3	19931223
AU 1994-70267	A3	19940815
US 1995-427502	B1	19950424

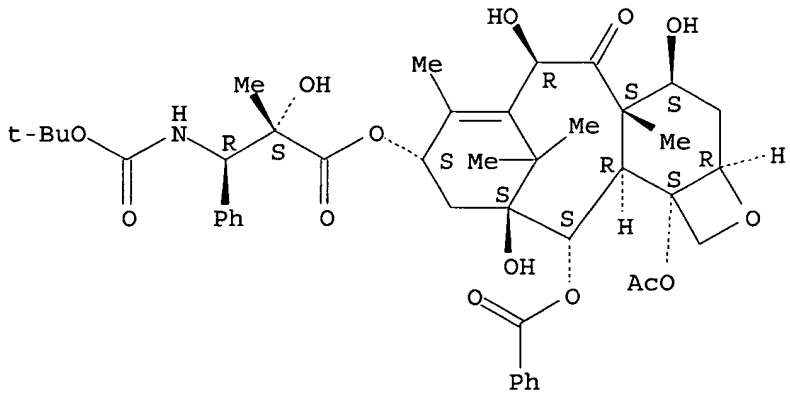
methyldocetaxel)
RN 168416-36-2 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-α-methyl-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **168416-30-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(novel niobium chloride-based stereoselective approach to methyldocetaxel)
RN 168416-30-6 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-α-methyl-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



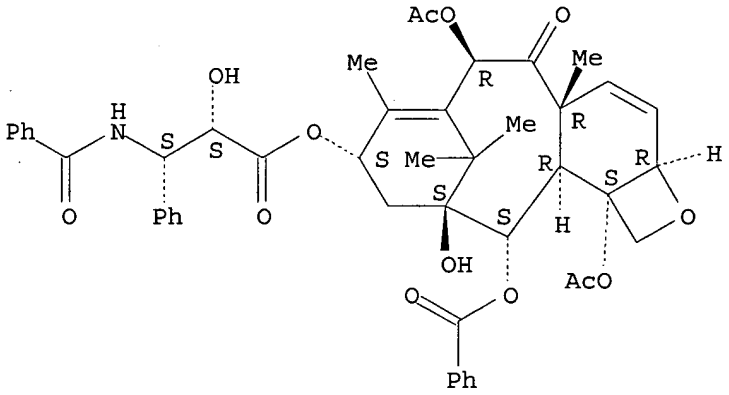
AB Taxane derivs. I (R1 = OR or R; R = C1-C6 alkyl, C2-C5 alkenyl; R2 = H or Ac), modified in the 6-7 positions, are antitumor agents. A procedure for the preparation of I and their 2'-epimers is also claimed.

IT **172586-63-9P**, 7-Deoxy-2'-epi-taxol-6-ene
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of unsatd. taxane derivs. as antitumor agents)

RN 172586-63-9 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,4a,5,6,9,10,11,12,12a,12b-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4aβ,6β,9α(αS*,βS*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 37 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:722745 CAPLUS

DOCUMENT NUMBER: 123:228561

TITLE: Docetaxel (taxotere) derivatives: novel NbCl3-based stereoselective approach to 2'-methyldocetaxel

AUTHOR(S): Denis, Jean-Noel; Fkyerat, Abdellatif; Gimbert, Yves; Coutterez, Claire; Mantellier, Pierre; Jost, Sylvie; Greene, Andrew E.

CORPORATE SOURCE: LEDSS, Univ. J. Fourier, Grenoble, 38041, Fr.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1995), (14), 1811-15
CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

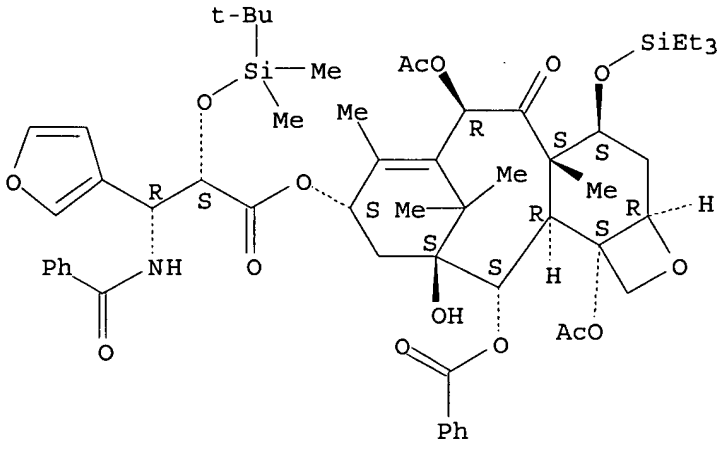
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:228561

AB The C-2 methylated 2S,3R and 2R,3S side chains of docetaxel have been enantioselectively prepared and esterified with protected 10-deacetylbaccatin III to provide novel analogs of docetaxel.

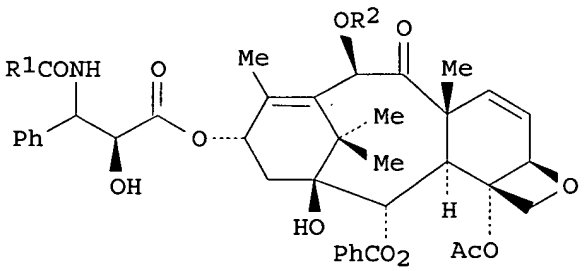
IT **168416-36-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel niobium chloride-based stereoselective approach to



L51 ANSWER 36 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:998252 CAPLUS
DOCUMENT NUMBER: 124:87428
TITLE: Unsaturated taxane derivatives.
INVENTOR(S): Mongelli, Nicola; Menichincheri, Maria; Fusar Bassini, Domenico; Ciomei, Marina
PATENT ASSIGNEE(S): Pharmacia S.p.A., Italy
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 19516631	A1	19951116	DE 1995-19516631		19950505
GB 2289277	A1	19951115	GB 1995-9353		19950509
GB 2289277	B2	19980819			
JP 07304761	A2	19951121	JP 1995-110678		19950509
PRIORITY APPLN. INFO.:			GB 1994-9131	A	19940509

OTHER SOURCE(S): CASREACT 124:87428; MARPAT 124:87428
GI



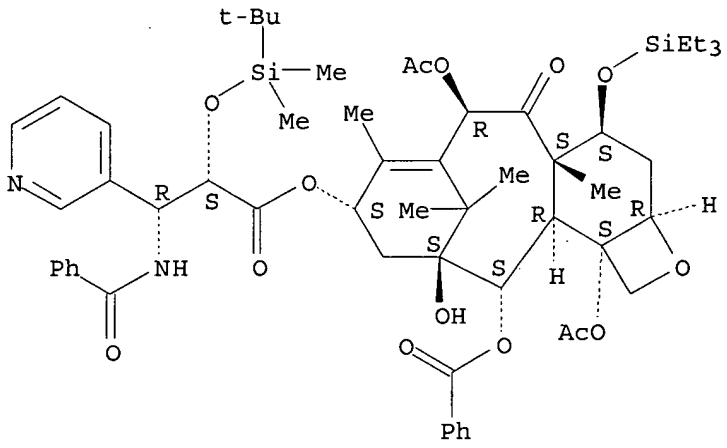
I

pentyl), and N-debenzoyl-N-(3-furoyl)paclitaxel (IV; R2 = 3-furyl) were found to be more cytotoxic than paclitaxel against this cell line. 3'-Dephenyl-3'-(4-pyridyl)paclitaxel (II; R = 4-pyridyl) and N-debenzoyl-N-(2-furoyl)paclitaxel (IV; R2 =2-furyl) displayed cytotoxicity against B16 melanoma cells similar to paclitaxel.

IT **158412-29-4P 158412-30-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis, conformational anal., and biol. evaluation of heteroarom. taxanes)

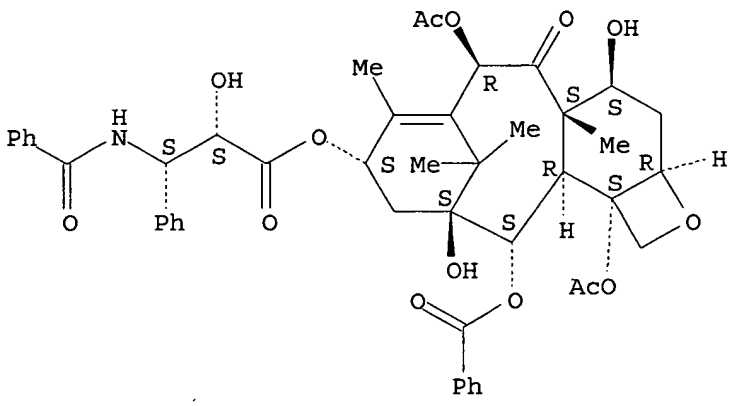
RN 158412-29-4 CAPLUS
CN 3-Pyridinepropanoic acid, β-(benzoylamino)-α-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 158412-30-7 CAPLUS
CN 3-Furanpropanoic acid, β-(benzoylamino)-α-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 35 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:191997 CAPLUS
DOCUMENT NUMBER: 124:317514
TITLE: Synthesis, Conformational Analysis, and Biological Evaluation of Heteroaromatic Taxanes
AUTHOR(S): Georg, Gunda I.; Harriman, Geraldine C. B.; Hepperle, Michael; Clowers, Jamie S.; Vander Velde, David G.; Himes, Richard H.
CORPORATE SOURCE: Department of Medicinal Chemistry, University of Kansas, Lawrence, KS, 66045, USA
SOURCE: Journal of Organic Chemistry (1996), 61(8), 2664-76
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:317514
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The asym. syntheses of heteroarom. 3-[(tert-butyldimethylsilyl)oxy]-2-azetidinones I (R = 2-, 3-, 4-pyridyl, 2-, 3-furyl) via chiral ester enolate-imine cyclocondensation chemical are described. The azetidinones contain heteroarom. moieties which, in certain cases, contribute to a decrease in enantioselectivity due to possible alternate coordinations in the transition states. The (3R,4S)-3-[(tert-butyldimethylsilyl)oxy]-4-heteroaryl-2-azetidinones I were subsequently converted to the heteroarom. taxanes II and III (R1 = OCMe3, pentyl, nonyl). Conformational analyses of the 3'-(2-pyridyl) analog II (R = 2-pyridyl) and 3'-(2-furyl) analog III (R1 = OCMe3) indicate they have solution conformational preferences virtually identical to paclitaxel and docetaxel. Heteroarom. N-acyl paclitaxel analogs IV (R2 = 2-, 3-, 4-pyridyl, 2-, 3-furyl) were prepared from N-debenzoylpaclitaxel via Schotten-Baumann acylation. The majority of the 14 analogs displayed good to excellent activity in a microtubule assembly assay in comparison to paclitaxel. The analogs were also tested for cytotoxicity against B16 melanoma cells. 3'-Dephenyl-3'-(2-pyridyl)paclitaxel (II; R = 2-pyridyl), 3'-dephenyl-3'-(2-furyl)paclitaxel (II; R = 2-furyl), N-BOC-3'-dephenyl-3'-(2-furyl)paclitaxel (III; R = OCMe3), 3'-dephenyl-3'-(2-furyl)-N-(hexanoyl)paclitaxel (III; R1 =

AUTHOR(S): Cabri, Walter
CORPORATE SOURCE: Chemical Res. & Development, Bristol-Myers Squibb, Sermoneta, 04010, Italy
SOURCE: Tetrahedron Letters (1996), 37(27), 4785-4786
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:143070

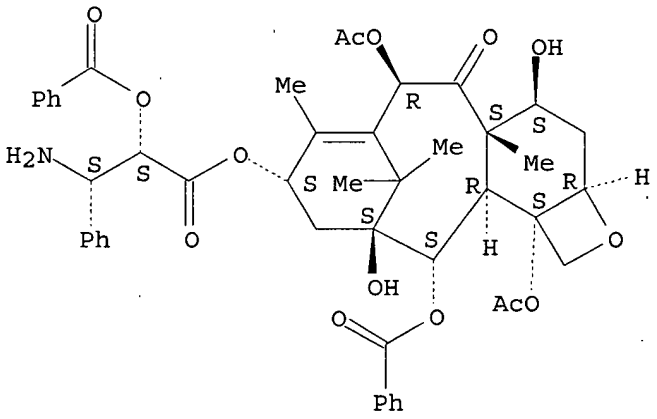
AB A new 2-step synthesis of 2'-epi-Taxol starting from natural Taxol is described. The approach is centered on the formation of oxazoline on the side chain with concomitant inversion of C-2' followed by acid hydrolysis.

IT **179551-57-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(high yield semisynthetic approach to 2'-epi-taxol)

RN 179551-57-6 CAPLUS

CN Benzenepropanoic acid, β-amino-α-(benzoyloxy)-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, hydrochloride, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

IT **179798-21-1P**, 2'-epi-Taxol
RL: SPN (Synthetic preparation); PREP (Preparation)
(high yield semisynthetic approach to 2'-epi-taxol)

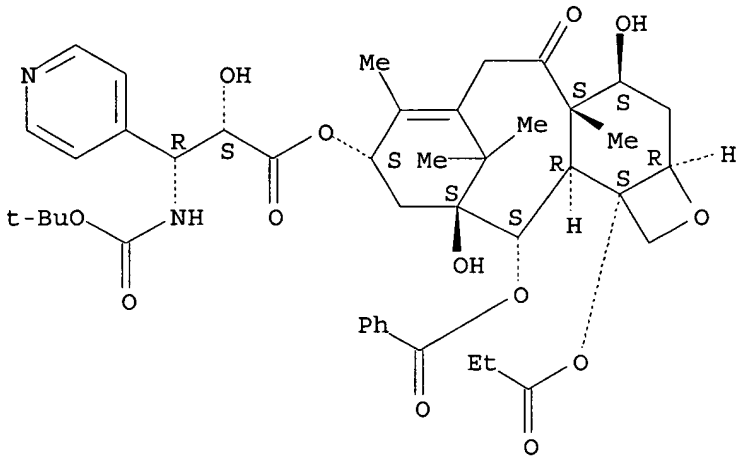
RN 179798-21-1 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

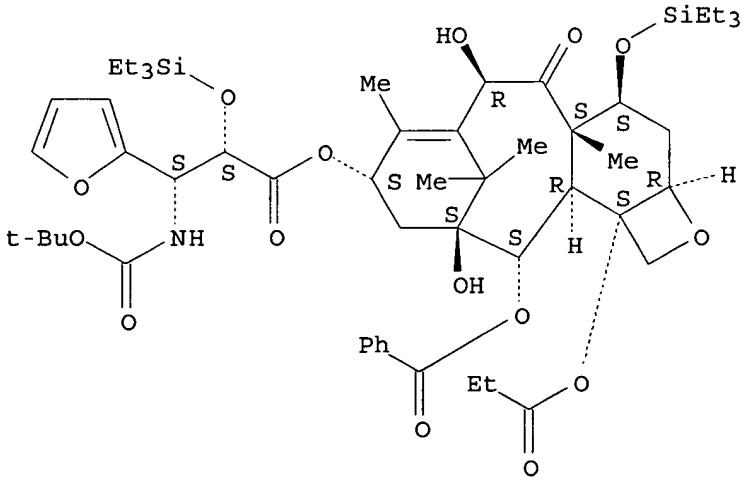
dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 184760-09-6 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-6,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxopropoxy)-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

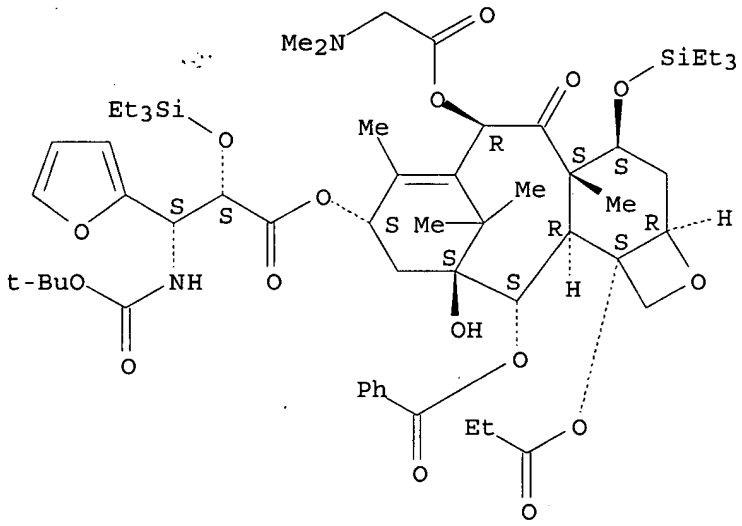
Absolute stereochemistry.



L51 ANSWER 34 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:427283 CAPLUS
DOCUMENT NUMBER: 125:143070
TITLE: A high yield semisynthetic approach to 2'-epi-Taxol

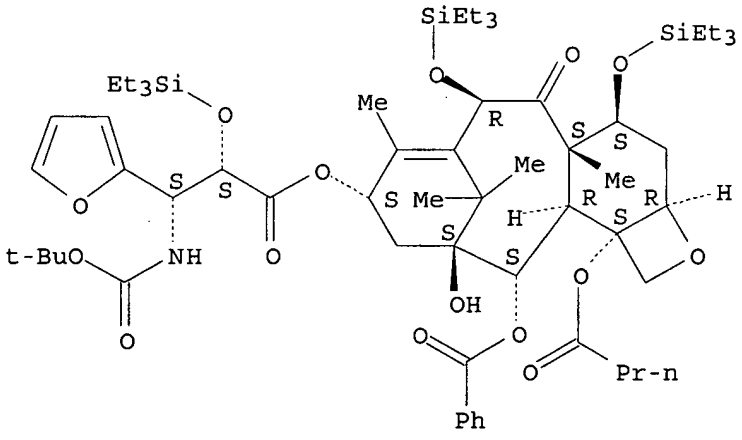
(benzoyloxy)-9-[(2S,3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-1-oxo-2-[(triethylsilyl)oxy]propoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxopropoxy)-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 184760-07-4 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxobutoxy)-4,6-bis[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

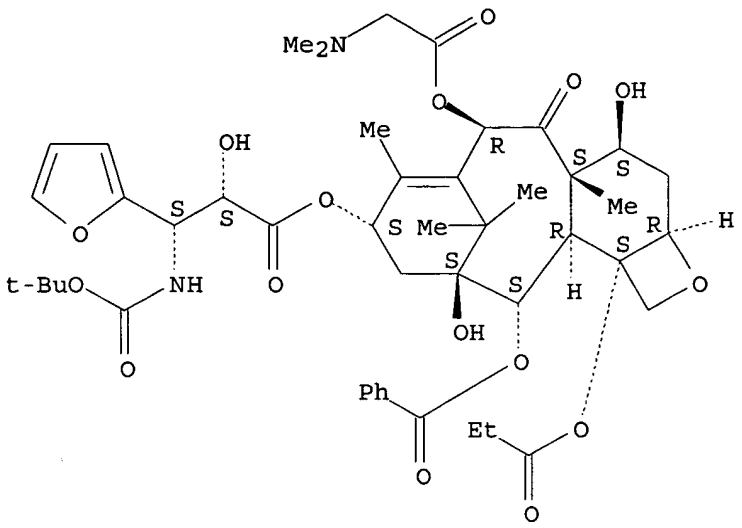
Absolute stereochemistry.



RN 184760-08-5 CAPLUS
CN 4-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-

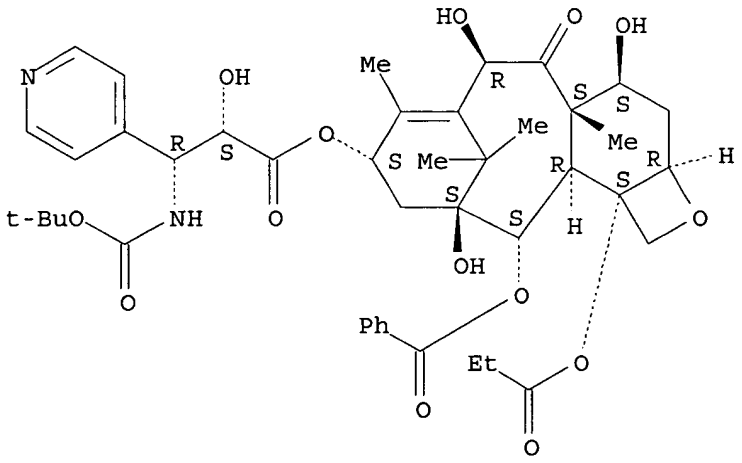
NAME)

Absolute stereochemistry.



RN 184864-49-1 CAPLUS
CN 4-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

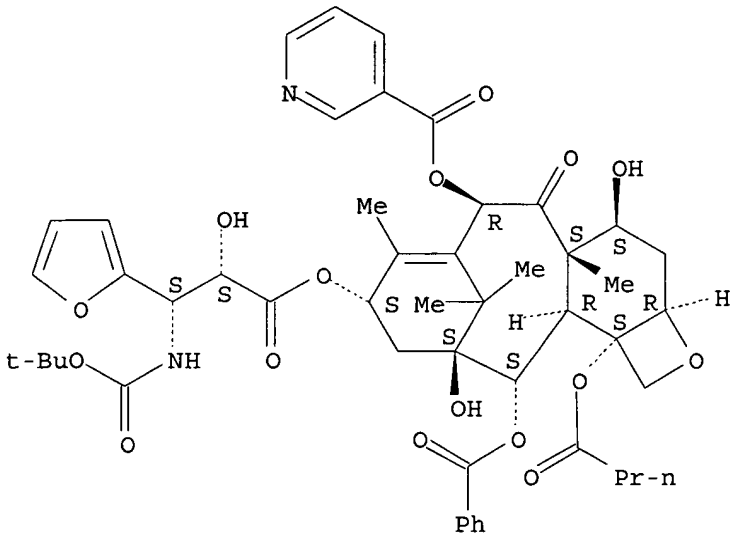
Absolute stereochemistry.



IT **184760-06-3P 184760-07-4P 184760-08-5P 184760-09-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of baccatin III derivs. as antitumors)
RN 184760-06-3 CAPLUS
CN Glycine, N,N-dimethyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12-

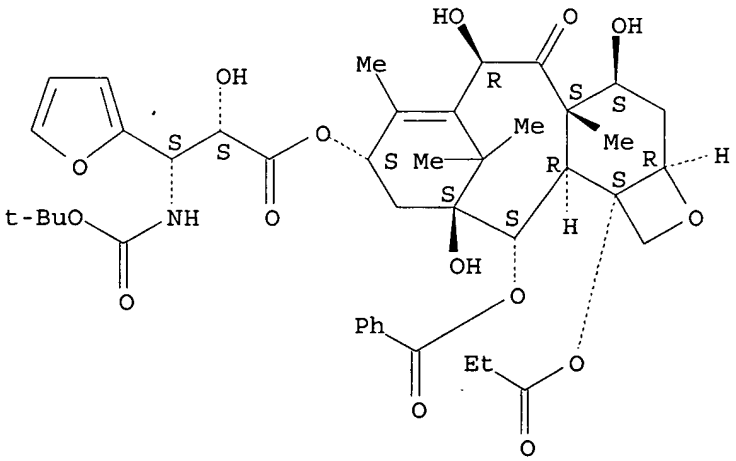
b]oxet-6-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2S*,3 S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 184760-03-0 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



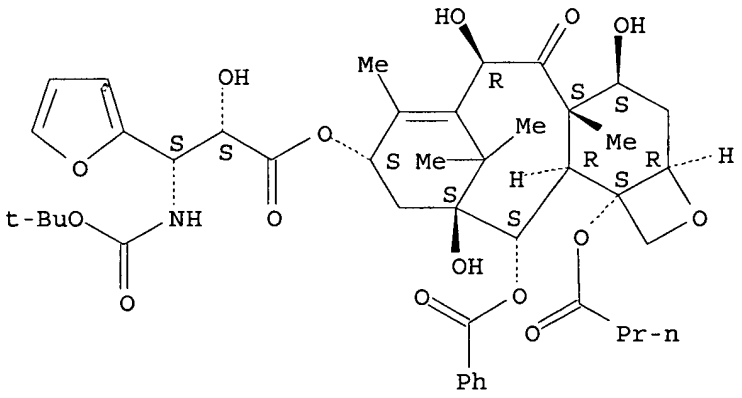
RN 184760-04-1 CAPLUS
CN Glycine, N,N-dimethyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12-(benzoyloxy)-9-[(2S,3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-2-hydroxy-oxopropoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of baccatin III derivs. as antitumors)

RN 184759-99-7 CAPLUS

CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxobutoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11.alpha.,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

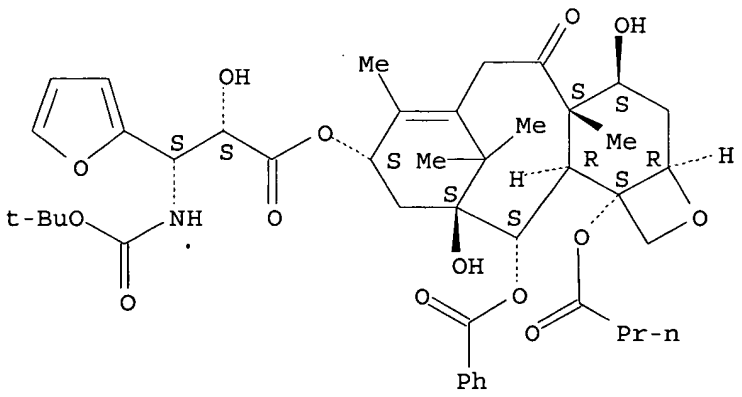
Absolute stereochemistry.



RN 184760-01-8 CAPLUS

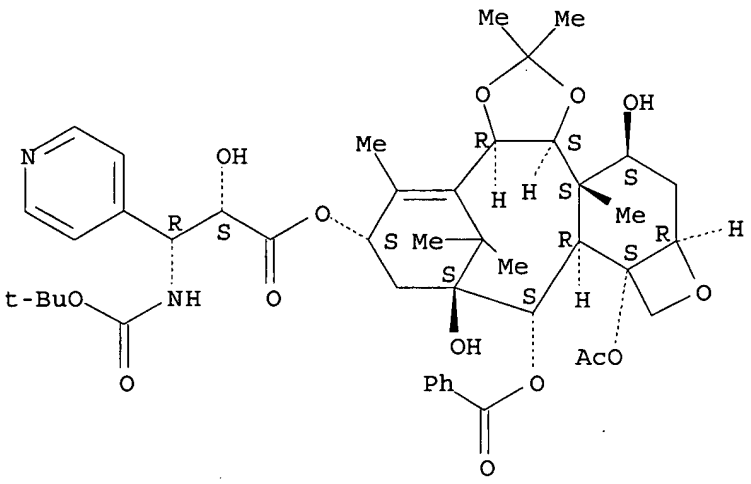
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxobutoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 184760-02-9 CAPLUS

CN 3-Pyridinecarboxylic acid, 12-(benzoyloxy)-9-[3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-2-hydroxy-1-oxopropoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12b-(1-oxobutoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-



L51 ANSWER 33 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:20747 CAPLUS
DOCUMENT NUMBER: 126:60178
TITLE: Preparation of baccatin III derivatives as antitumors
INVENTOR(S): Terasawa, Hirofumi; Soga, Tsunehiko; Uoto, Koichi
PATENT ASSIGNEE(S): Daiichi Seiyaku Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 57 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

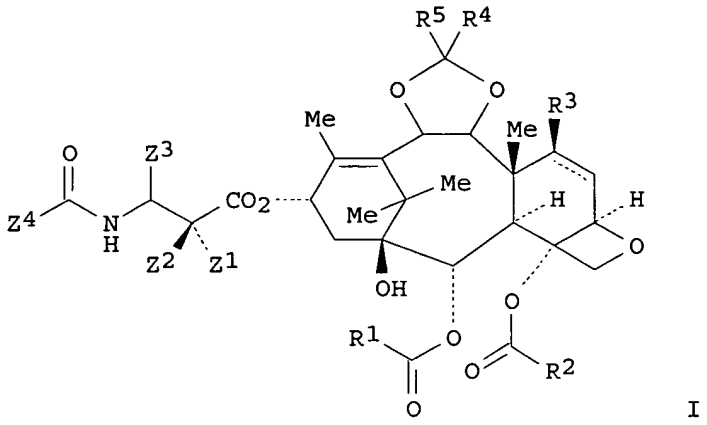
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08253465	A2	19961001	JP 1995-58508	19950317
PRIORITY APPLN. INFO.:			JP 1995-58508	19950317
OTHER SOURCE(S):	MARPAT 126:60178			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; R1 = (un)substituted alkyl, etc.; R2 = H, (un)substituted alkyl, etc.; R3 = H, OH, -CO-R9, etc.; R9 = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, etc.; R4 = H, OH, halo, alkyl; R5 = H, halo, alkyl; R6 = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, etc.; R7 = alkyl, aryl, alkoxy; R8 = H, OH] and their pharmaceutically acceptable salts, useful as antitumors, are prepared Thus, II was prepared in 5 steps from 10-deacetyl-7,10-bis-O-(triethylsilyl)baccatin III via oxidation, alkylation with MeI, reduction, reaction with (2S,3S)-N-(tert-butoxycarbonyl)-N,O-isopropylidene-3-phenylisoserine, and desilylation. In an in vitro study, II had a GI50 0.260 ng/mL against mouse leukemia cells P388.

IT **184759-99-7P 184760-01-8P 184760-02-9P**
184760-03-0P 184760-04-1P 184864-49-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological



I

AB The title compds. [I; R1 = (un)substituted phenyl; R2 = alkyl, alkenyl, alkynyl, cycloalkyl or alkoxy; R3 = H, OH, halo, alkoxy, -CO-R31, etc.; R31 = alkylamino, alkenyl, alkynyl, cycloalkyl, aryl or a heterocycle; R4, R5 = H, alkyl, alkenyl, alkynyl, aryl, heterocyclyl; Z1 = H, OH, halo, alkyl; Z2 = H, OH, halo or alkyl; Z3 = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, etc.; Z4 = alkyl, aryl, alkoxy, etc.] and their pharmaceutically acceptable salts, useful as antitumors, are prepared Thus, 10-deacetylbaccatin III was converted into 9β,13-O-[(2R,3R)-3-(tert-butoxycarbonylamino)-3-(2-furyl)-2-hydroxypropionyl]-10-deacetyl-9-deacetyl-9-dihydro-9,10-O-isopropylidenebaccatin III via the intermediates 9β-10-deacetyl-9-dihydrobaccatin III, 9β-10-deacetyl-9-dihydro-9,10-O-isopropylidenebaccatin III, and 9β-13-O-[(2R,3R)-3-(tert-butoxycarbonylamino)-3-(2-furyl)-2-(triisopropylsilyloxy)propionyl]-10-deacetyl-9-dihydro-9,10-O-isopropylidenebaccatin III. In an in vitro study, I [R1 = Ph, R2 = Pr, R3 = β-OH, R4 = morpholinomethyl, Z1 = OH, Z2 = H, Z3 = 2-furyl, Z4 = tert-butoxy] (also prepared) had an IC50 of 4.36 ng/mL against mouse leukemia cells P388.

IT **184759-16-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of baccatin III derivs. as antitumors)

RN 184759-16-8 CAPLUS

CN 4-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, 2a-(acetyloxy)-3-(benzoyloxy)-2a,2b,3,4,5,6,8a,11a,11b,12,13,13a-dodecahydro-4,12-dihydroxy-7,10,10,11b,14,14-hexamethyl-4,8-methano-2H-oxeto[3'',2'':3',4']benzo[1',2':3,4]cyclodeca[1,2-d][1,3]dioxol-6-yl ester, [2aS-[2aα,2bα,3α,4α,6α(αR*,βS*),8a.alpha.,11aα,11bβ,12β,13aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9633998	A1	19961031	WO 1996-JP1145	19960425
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2219675	AA	19961031	CA 1996-2219675	19960425
AU 9655145	A1	19961118	AU 1996-55145	19960425
AU 704198	B2	19990415		
EP 826688	A1	19980304	EP 1996-912252	19960425
EP 826688	B1	20010905		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, EE, SI, LT, LV, FI				
CN 1188477	A	19980722	CN 1996-194915	19960425
CN 1094940	B	20021127		
BR 9608040	A	19990112	BR 1996-8040	19960425
AT 205213	E	20010915	AT 1996-912252	19960425
ES 2164241	T3	20020216	ES 1996-912252	19960425
PT 826688	T	20020228	PT 1996-912252	19960425
TW 480262	B	20020321	TW 1996-85104983	19960425
JP 09012578	A2	19970114	JP 1996-106615	19960426
JP 3746563	B2	20060215		
NO 9704912	A	19971229	NO 1997-4912	19971024
NO 321942	B1	20060724		
US 6075140	A	20000613	US 1998-945276	19980205
HK 1008529	A1	20020328	HK 1998-109471	19980728
US 6211363	B1	20010403	US 2000-513852	20000225
US 2001041796	A1	20011115	US 2001-759378	20010116
US 6545151	B2	20030408		
US 2003162971	A1	20030828	US 2002-126653	20020422
US 6646123	B2	20031111		

PRIORITY APPLN. INFO.:	JP 1995-106295	A	19950428
	WO 1996-JP1145	W	19960425
	US 1998-945276	A1	19980205
	US 2000-513852	A1	20000225
	US 2001-759378	A3	20010116

OTHER SOURCE(S): MARPAT 126:60179
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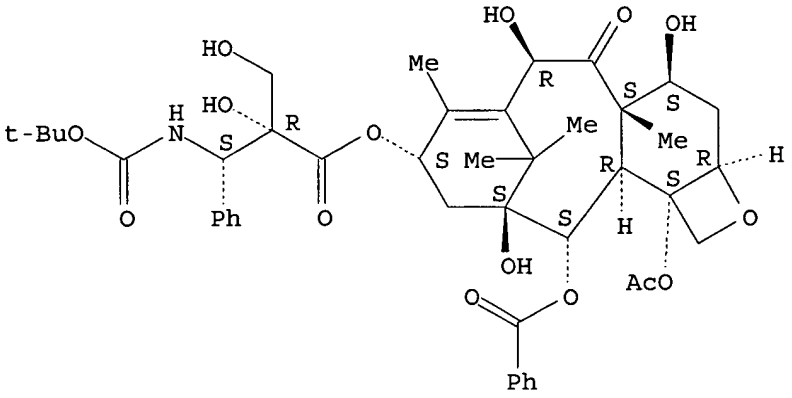
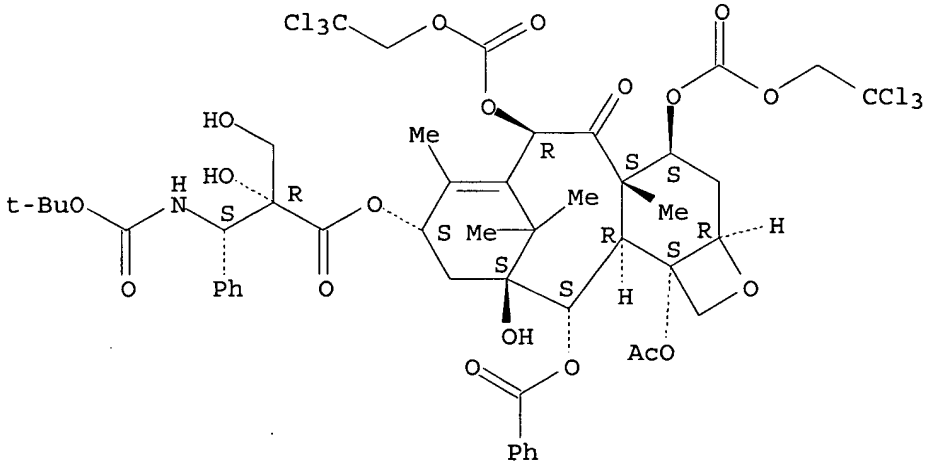


IT **186371-29-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. Baylis-Hillman-like reaction to prepare α-aminoalkylacrylic acid derivs. in synthesis of docetaxel hydroxymethyl analogs)
RN 186371-29-9 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-α-(hydroxymethyl)-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αR*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 32 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:33889 CAPLUS
DOCUMENT NUMBER: 126:60179
TITLE: Preparation of baccatin III derivatives as antitumors
INVENTOR(S): Terasawa, Hirofumi; Soga, Tsunehiko; Ishiyama, Takashi

ACCESSION NUMBER: 1997:56511 CAPLUS
DOCUMENT NUMBER: 126:131656
TITLE: Effective enantioselective approach to α-aminoalkylacrylic acid derivatives via a synthetic equivalent of an asymmetric Baylis-Hillman reaction: application to the synthesis of two C-2 hydroxymethyl analogs of docetaxel
AUTHOR(S): Genisson, Yves; Massardier, Christine; Gautier-Luneau, Isabelle; Greene, Andrew E.
CORPORATE SOURCE: LEDSS, Univ. Joseph Fourier, Grenoble, 38041, Fr.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1996), (24), 2869-2872
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:131656
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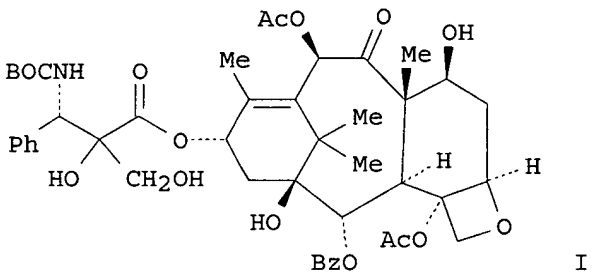

I

AB Two C-2' hydroxymethyl analogs I of docetaxel have been synthesized from 10-deacetylbaccatin III and enantiopure (3S)-3-(N-tert-butoxycarbonylamino)-2-methylene-3-phenylpropanoic acid. The latter was prepared via the use of a new method, the reductive condensation of a chiral propiolate with benzaldehyde imines. I have no significant cytotoxicity vs. KB or KB-V1, but the threo isomer did show more inhibition of microtubule depolymn. than the erythro.

IT **186371-30-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(asym. Baylis-Hillman-like reaction to prepare α-aminoalkylacrylic acid derivs. in synthesis of docetaxel hydroxymethyl analogs)

RN 186371-30-2 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-α-(hydroxymethyl)-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αR*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PRIORITY APPLN. INFO.: JP 1995-93741 19950419

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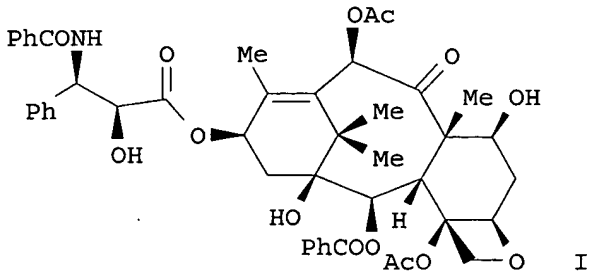


I

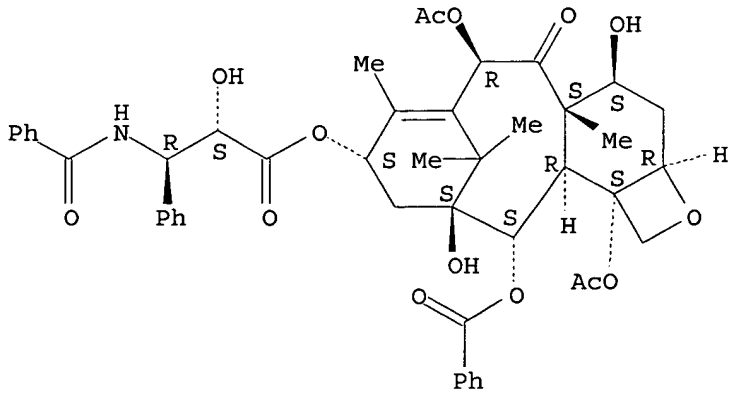
AB An antitumor compound NSC-LSC2 (I) is manufactured by culturing cells originate from Taxus sp., recovery of the cultured cells, and collection of I from the cells. New leaves of T. cuspidata were cultured in a solid Schenk-Hildebrandt (SH) medium (pH 5.8) containing NAA to 5 mg/L at 20° or 25° under light, subcultured in a liquid modified SH medium (pH 5.8) containing NAA to 5 mg/L, KNO3, (NH4)2SO4, and KH2PO4, the cells were dried, homogenized, extracted with MeOH-CH2Cl2 mixture, and the extract was fractionated and subjected to HPLC to purify I. I inhibited KB cells (human carcinoma cell line) with IC50 of 10 ng/mL.

IT **149197-23-9P**, NSC-LSC 2
RL: BAC (Biological activity or effector, except adverse); BMF (Bioindustrial manufacture); BOC (Biological occurrence); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(manufacture of antitumor NSC-LSC2 by cell culture of Taxus)

RN 149197-23-9 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 31 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

PRIORITY APPLN. INFO.: US 1995-523443 A 19950905

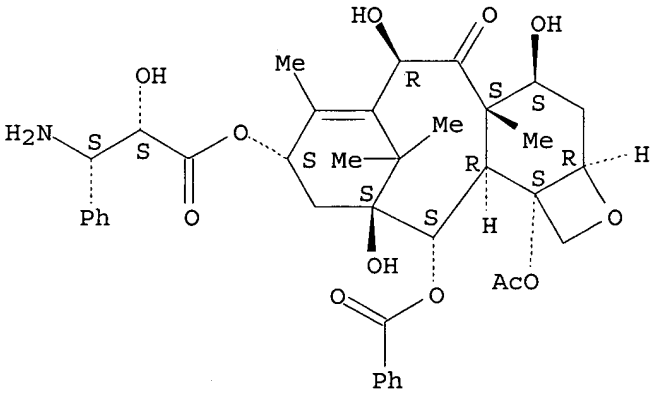
AB A process for the separation of taxanes, particularly taxol, cephalomannine, baccatin III, and deacetylbaccatin III, from ornamental yew tissue is described. The process involves a specific solvent mixture of water and 50-95% MeOH, EtOH, or acetone and treatment of the resulting extract using activated C, preferably charcoal. The taxanes are preferably separated from the crude extract by a normal phase chromatog. step which preferably is through vacuum and then medium pressure column chromatog. separation, using inexpensive silica gel as an absorbent. The silica gel is regenerated by heating in a furnace above .apprx.500° to remove adsorbed organic materials.

IT **133577-37-4P**
RL: BMF (Bioindustrial manufacture); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(isolation and purification of taxol and taxanes from Taxus spp.)

RN 133577-37-4 CAPLUS

CN Benzenepropanoic acid, β-amino-α-hydroxy-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βS*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L51 ANSWER 30 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:72099 CAPLUS

DOCUMENT NUMBER: 126:88340

TITLE: Antitumor compound NSC-LSC2 and its manufacture by cell culture of Taxus

INVENTOR(S): Takigawa, Kenji; Takami, Masamichi; Asari, Tooru; Fukumoto, Kenji

PATENT ASSIGNEE(S): Shinnippon Seitetsu KK, Japan; Shinnittetsu Kagaku

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08291062	A2	19961105	JP 1995-93741	19950419

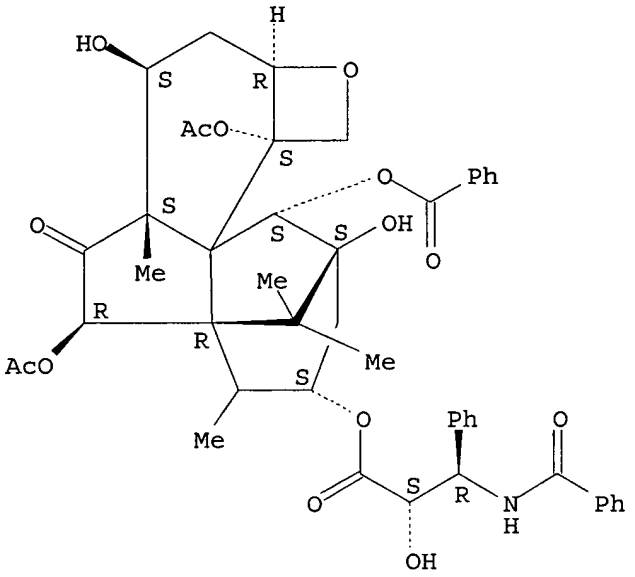
discovery through development. This library of paclitaxel degradation derivs. provides a foundation for future development work regarding product monitoring, as well as use as a diagnostic tool for new degradation products.

IT **194148-31-7**
RL: ANT (Analyte); ANST (Analytical study)
(determination of paclitaxel degradation derivs. in bulk drug by HPLC and mass
spectrometry)

RN 194148-31-7 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, 2a,8-bis(acetyloxy)-3-(benzoyloxy)dodecahydro-4,10-dihydroxy-7,9a,12,12-tetramethyl-9-oxo-3H-4,7a-methanocyclohept[3,3a]indeno[5,4-b]oxet-6-yl ester, [2aS,3S,4S,6S(αS,βR),7aR,8R,9aS,10S,11aR]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

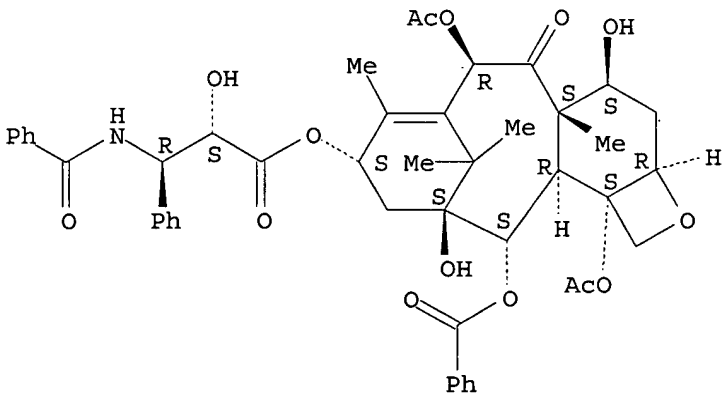


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 29 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:267272 CAPLUS
DOCUMENT NUMBER: 126:255480
TITLE: Process for the isolation and purification of taxol and taxanes from Taxus spp
INVENTOR(S): Nair, Muraleedharan G.
PATENT ASSIGNEE(S): Michigan State University, USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9709443	A1	19970313	WO 1996-US13212	19960815

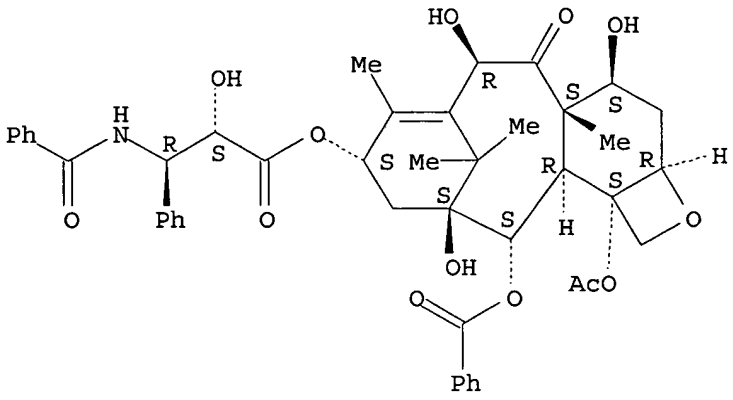
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

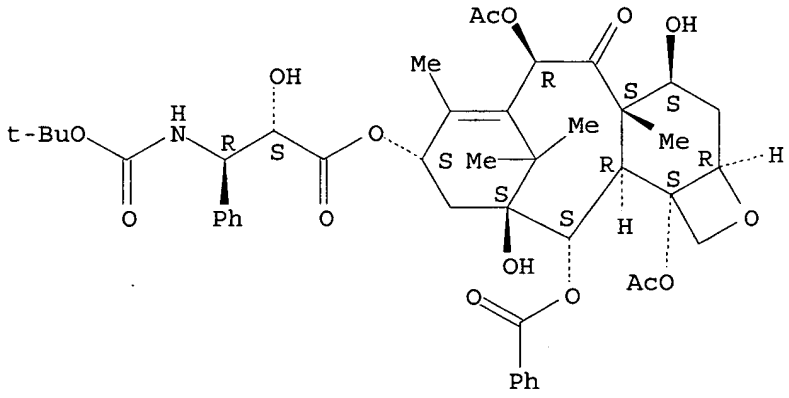
L51 ANSWER 28 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:469237 CAPLUS
DOCUMENT NUMBER: 127:195561
TITLE: Profiling degradants of paclitaxel using liquid chromatography-mass spectrometry and liquid chromatography-tandem mass spectrometry substructural techniques
AUTHOR(S): Volk, Kevin J.; Hill, Susan E.; Kerns, Edward H.; Lee, Mike S.
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, 5 Research Parkway, P.O. Box, 5100, Wallingford, CT, 06492, USA
SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1997), 696(1), 99-115
CODEN: JCBBEP; ISSN: 0378-4347
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A rapid and systematic strategy based on liquid chromatog.-mass spectrometry (LC-MS) profiling and liquid chromatog.-tandem mass spectrometry (LC-MS-MS) substructural techniques was utilized to elucidate the degradation products of paclitaxel, the active ingredient in Taxol. This strategy integrates, in a single instrumental approach, anal. HPLC, UV detection, full-scan electrospray MS, and MS-MS to rapidly and accurately elucidate structures of impurities and degradation derivs.. In these studies, degradation derivs. induced by acid, base, peroxide, and light were profiled using LC-MS and LC-MS-MS methodologies resulting in an LC-MS degradant database which includes information on mol. structures, chromatog. behavior, mol. mass, and MS-MS substructural information. The stressing conditions which may cause drug degradation are utilized to validate the anal. monitoring methods and serve as predictive tools for future formulation and packaging studies. Degradation products formed upon exposure to basic conditions included baccatin III, paclitaxel side chain Me ester, 10-deacetylpaclitaxel, and 7-epipaclitaxel. Degradation products formed upon exposure to acidic conditions included 10-deacetylpaclitaxel and the oxetane ring opened product. Treatment with hydrogen peroxide produced only 10-deacetylpaclitaxel. Exposure to high intensity light produced a number of degradation derivs.. The most abundant photodegradant of paclitaxel corresponded to an isomer which contains a C3-C11 bridge. These methodologies are applicable at any stage of the drug product cycle from



RN 125354-17-8 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149197-23-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

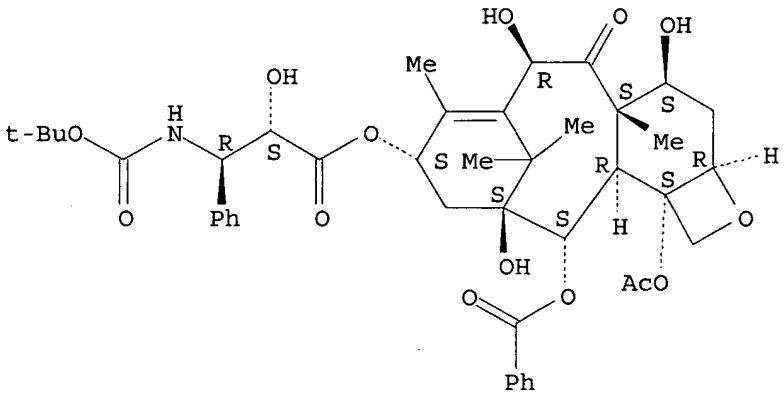
AB Using the method of stepwise multivariate linear regression (SMLR), the quant. structure-activity relationships (QSAR) of two isomeric series of taxol and its derivs. were studied. The molar refractivity of the C3' substituent of the C13 side chain showed significant correlation with its activity. The results suggest that structural changes in the C3' substituents may be critical to the anticancer function.

IT **114977-29-6 125354-13-4 125354-17-8 149197-23-9**
RL: PRP (Properties)
(QSAR of taxol and its derivs. based on stepwise multivariate linear regression anal.)

RN 114977-29-6 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

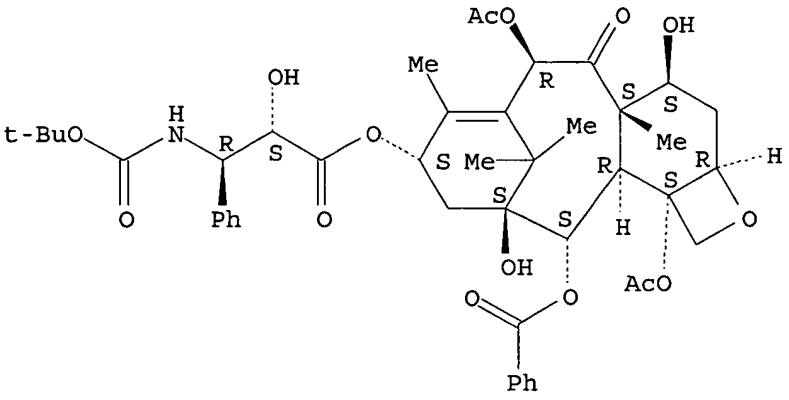
Absolute stereochemistry.



RN 125354-13-4 CAPLUS

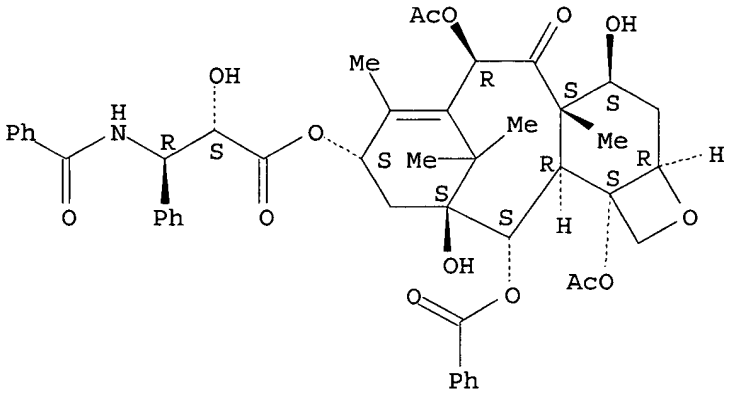
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149197-23-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 27 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:578023 CAPLUS
DOCUMENT NUMBER: 127:234448
TITLE: Study on QSAR of taxol and its derivatives based on stepwise multivariate linear regression analysis
AUTHOR(S): Liu, Ailin; Chi, Hanlin
CORPORATE SOURCE: Inst. Materia Medica, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Journal of Chinese Pharmaceutical Sciences (1997), 6(1), 18-22
CODEN: JCHSE4; ISSN: 1003-1057
PUBLISHER: Beijing Medical University, School of Pharmaceutical Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

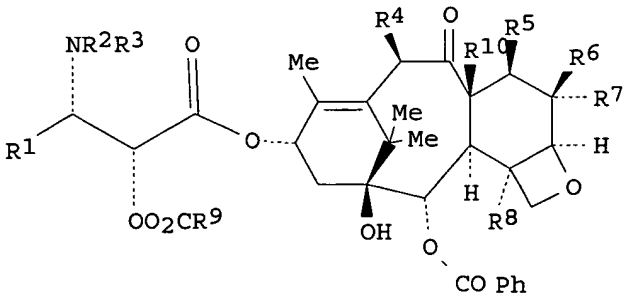
TITLE: Comparative Molecular Field Analysis of A Series of Paclitaxel Analogs
AUTHOR(S): Zhu, Qiqing; Guo, Zongru; Huang, Niu; Wang, Minmin; Chu, Fengming
CORPORATE SOURCE: Department of Synthetic Medicinal Chemistry Institute of Materia Medica Chinese Academy of Medical Sciences, Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Journal of Medicinal Chemistry (1997), 40(26), 4319-4328
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of 94 paclitaxel analogs exhibiting antitumor activity by promoting the assembly of microtubules and inhibiting the disassembly process of microtubules to tubulin were investigated using the comparative mol. field anal. (CoMFA) method. These compds. belonging to 10 structural classes were randomly divided into a training set of 80 compds. and a test set of 14 compds. Since the 3-dimensional structure of ligand-receptor complex is unknown, from x-ray and NMR data, the authors rationally selected the 3-dimensional structure of paclitaxel in a polar solution as the active conformation and starting structure for mol. modeling, the other mols. were aligned using this mol. model as the template. The most optimal CoMFA yielded a 2-component model, with significant cross-validation r2cv of 0.640 and conventional r2 of 0.868. The predictive ability of training set model was tested on the test set of 14 compds. The tests not only revealed the robustness of the CoMFA model but demonstrated that for this model r2pred based on the mean activity of test set compds. can accurately estimate external predictivity but r2pred based on the mean activity of training set compds. overestimated the model. The CoMFA model explained why the activity of taxoid is sensitive to the stereochem. of the atoms at C-2' and C-3' positions and the presence of hydroxyl group at C-2' position. The other factors affecting activity were also elucidated according to standard coefficient contour maps of steric and electrostatic fields derived from the CoMFA model.

IT **125354-17-8 149197-23-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(comparative mol. field anal. of paclitaxel analogs)

RN 125354-17-8 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



I

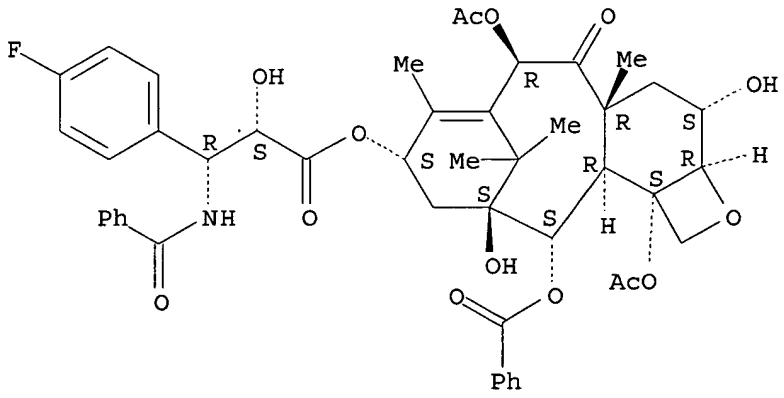
AB Taxane derivs. I [R1 = alkyl, cycloalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl; R2, R3 = H, sulfenamido; R4 = H, OH, Ac; R5 = H, OH, alkoxy, acyloxy, alkoxycarbonyloxy, carbamoyloxy; R6, R7 = H, OH, alkyl; R5R6 = O, bond, R7 = H; R8 = acyloxy, thioacyloxy; R9 = (un)substituted aryl, cycloalkyl, alkyl, heteroaryl; R10 = Me, CH2OH; R5R10 = CH2] were prepared The new derivs. are antitumor agents useful in the treatment of such cancers as ovarian, breast, lung, gastric, colon, head and neck, melanoma and leukemia. Thus, I [R1, R9 = Ph, R2, R3, R6, R7 = H, R4, R8 = OAc, R5 = OH, R10 = Me] was treated with 2-O2NC6H4SCl to give I [R2 = 2-O2NC6H4S, other R groups unchanged] which was active against M109 lung carcinoma in mice.

IT **214146-88-0P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of sulfenamide derivs. of paclitaxel as antitumor agents)

RN 214146-88-0 CAPLUS

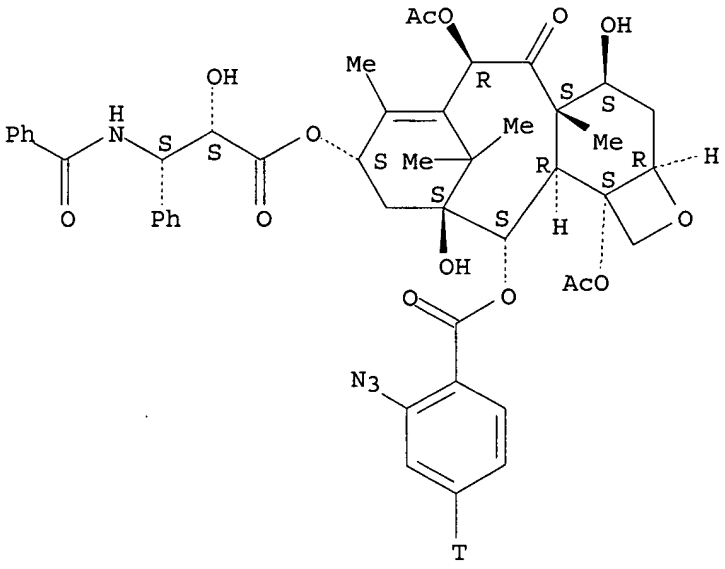
CN Benzenepropanoic acid, β-(benzoylamino)-4-fluoro-α-hydroxy-, (2aR,3S,4aR,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-3,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 26 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:31653 CAPLUS
DOCUMENT NUMBER: 128:30043

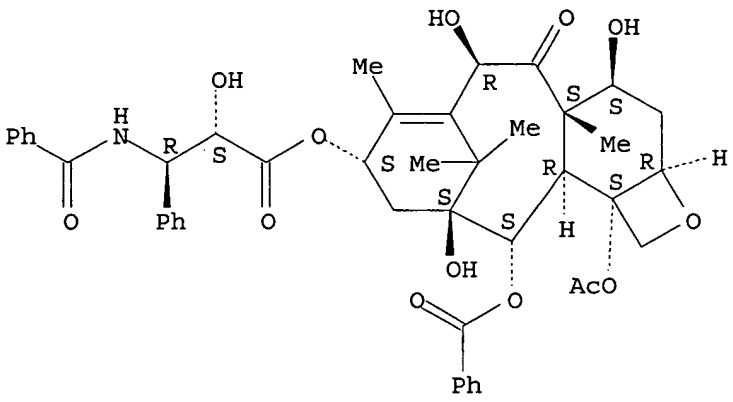


REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 25 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:668019 CAPLUS
DOCUMENT NUMBER: 129:290253
TITLE: Sulfenamide taxane derivatives
INVENTOR(S): Scola, Paul M.; Vyas, Dolatrai M.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: U.S., 29 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5821263	A	19981013	US 1997-902451	19970729

PRIORITY APPLN. INFO.: US 1997-902451 19970729
OTHER SOURCE(S): MARPAT 129:290253
GI



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

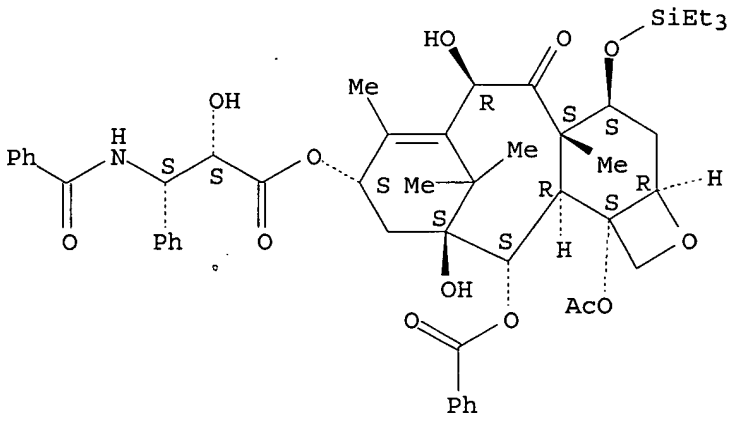
L51 ANSWER 24 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:5360 CAPLUS
DOCUMENT NUMBER: 130:206928
TITLE: Photoaffinity labeling approach to map the taxol-binding site on the microtubule
AUTHOR(S): Orr, George A.; Rao, Srinivasa; Swindell, Charles S.; Kingston, David G. I.; Horwitz, Susan Band
CORPORATE SOURCE: Albert Einstein College of Medicine, Bronx, NY, 10461, USA
SOURCE: Methods in Enzymology (1998), 298(Molecular Motors and the Cytoskeleton, Part B), 238-252
CODEN: MENZAU; ISSN: 0076-6879
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Photoaffinity labeling studies of the interaction of taxol with tubulin were done using the taxol analogs with an arylazide substituent attached to either the C-3' of the A ring side chain or the C-2 of the B ring of the taxoid nucleus. Details of the labeling of microtubules with the photoreactive taxol analogs, isolation of β-tubulin and determination of the binding sites on tubulin are outlined. (c) 1998 Academic Press.

IT **220916-61-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(photoaffinity labeling approach to map the taxol-binding site on the microtubule using arylazide derivs. of taxol)

RN 220916-61-0 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-[(2-azidobenzoyl-4-t)oxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 23 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:322978 CAPLUS
DOCUMENT NUMBER: 131:124926
TITLE: A Unified and Quantitative Receptor Model for the Microtubule Binding of Paclitaxel and Epothilone
AUTHOR(S): Wang, Minmin; Xia, Xiaoyang; Kim, Yohan; Hwang, David; Jansen, Johanna M.; Botta, Maurizio; Liotta, Dennis C.; Snyder, James P.
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (1999), 1(1), 43-46
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Paclitaxel and epothilone represent the two major classes of antimicrotubule agents that promote tubulin polymerization and, presumably, mitotic arrest during cell division. A common minireceptor binding site model at β-tubulin has been constructed for these structurally divergent compds. Utilizing 20 amino acids identified in photoaffinity labeling expts., the 3-D model correlates measured and predicted Ki's with r = 0.99 and rms(ΔGcalc - ΔGexp) = 0.2 kcal/mol. In addition, the model predicts the affinity of compds. not used in the training set and explains much of the SAR for the paclitaxel and epothilone families.

IT **125354-13-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(A Unified and Quant. Receptor Model for the Microtubule Binding of Paclitaxel and Epothilone)

RN 125354-13-4 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

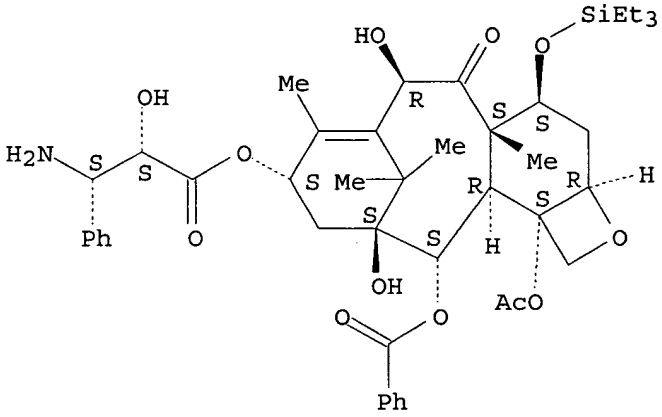
243-246
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:194518

AB A semisynthesis of paclitaxel has successfully been accomplished starting from a newly developed baccatin III derivative bearing a β-keto ester appendage on C-13.

IT **260249-50-1P 260261-02-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(semisynthesis of paclitaxel via a 10-deacetylbaccatin III derivative bearing a β-keto ester appendage)

RN 260249-50-1 CAPLUS
CN Benzenepropanoic acid, β-amino-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-6,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 260261-02-7 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-6,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

University, Tianjin, 300072, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2000), 21(3), 401-406
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

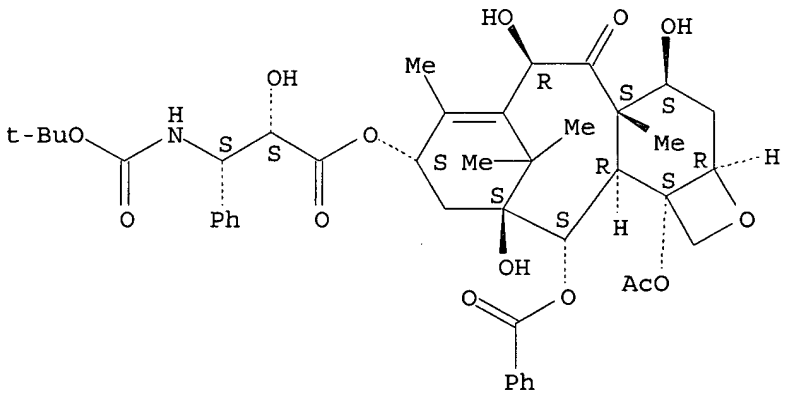
AB A series of 98 paclitaxel analogs were investigated using the comparative mol. field anal. (CoMFA) and a high predictive 3D-QSAR model with a significant cross-validated γcv2, conventional γ2, and predictive γpred.2 equaling to 0.714, 0.901, 0.812, resp., was obtained. It revealed that the changes of the C-13 side chain groups, especially 2'-OH, affected the activity significantly and others did less relatively. It also showed that the model was significant for the research and development of novel paclitaxel analogs to reduce the blind flight during drug designing.

IT **133577-33-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(studies on the quant. structure-activity relationships of paclitaxel analogs)

RN 133577-33-0 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

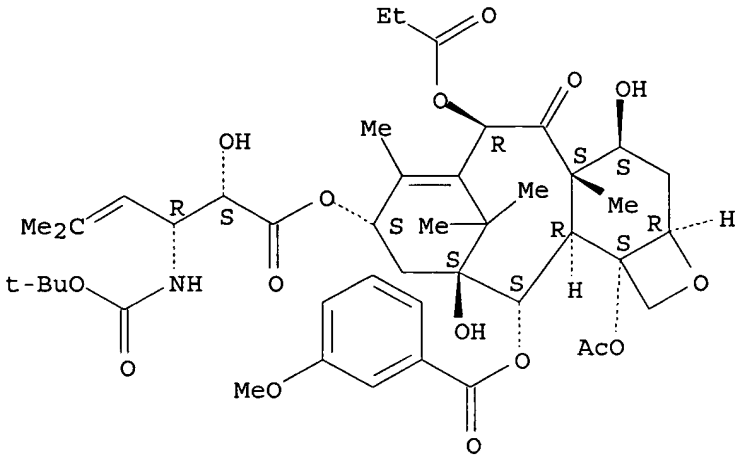
Absolute stereochemistry.



L51 ANSWER 22 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:42193 CAPLUS
DOCUMENT NUMBER: 132:194518
TITLE: A semisynthesis of paclitaxel via a 10-deacetylbaccatin III derivative bearing a β-keto ester appendage
AUTHOR(S): Mandai, Tadakatsu; Kuroda, Akiyoshi; Okumoto, Hiroshi; Nakanishi, Katsuyoshi; Mikuni, Katsuhiko; Ko-Ji, Hara; Ko-Zo, Hara
CORPORATE SOURCE: Department of Chemical Technology, Kurashiki University of Science and the Arts, Kurashiki, 712-8505, Japan
SOURCE: Tetrahedron Letters (1999), Volume Date 2000, 41(2),

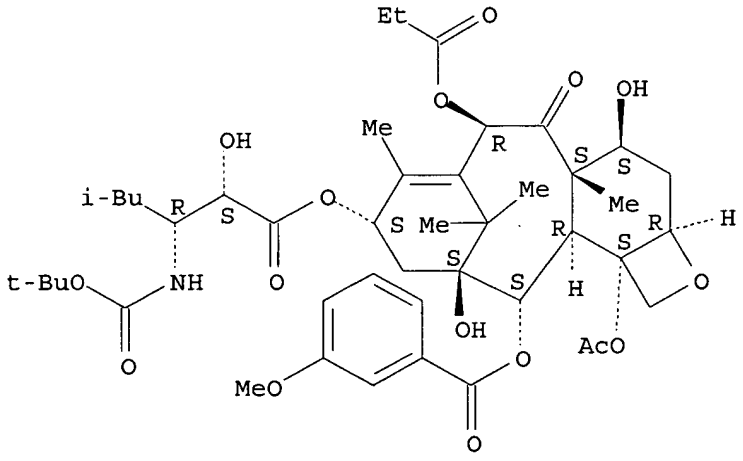
1H-cyclodeca[3,4]benz[1,2-b]oxet-12-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287180-37-4 CAPLUS
CN Benzoic acid, 3-methoxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-9-[[(2S,3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-1-oxohexyl]oxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

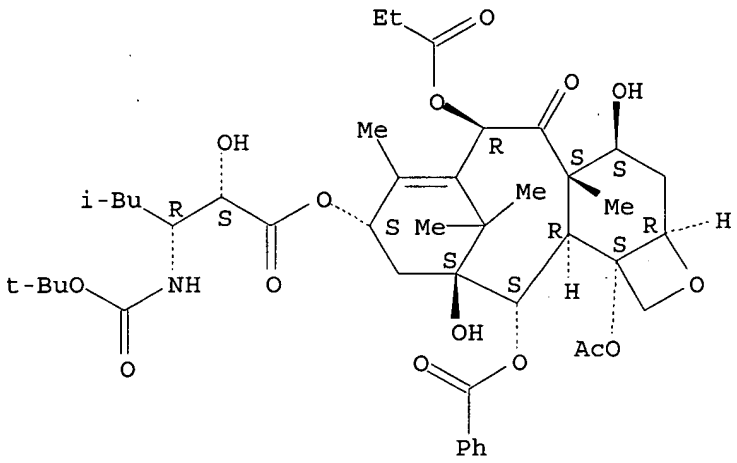


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 21 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:218668 CAPLUS
DOCUMENT NUMBER: 133:255
TITLE: Studies on the quantitative structure-activity relationships of paclitaxel analogs
AUTHOR(S): Shi, Bing-Xing; Liang, Shi-Le; Yuan, Ying-Jin; Sun, Ming; Miao, Fang-Ming
CORPORATE SOURCE: Department of Biochemical Engineering, Tianjin

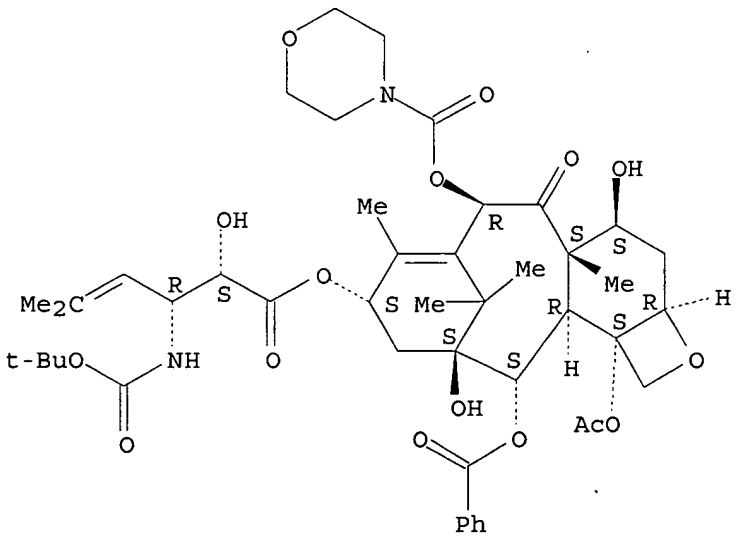
2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287180-35-2 CAPLUS
CN 4-Morpholinecarboxylic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-9-[[(2S,3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-1-oxo-4-hexenyl]oxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287180-36-3 CAPLUS
CN Benzoic acid, 3-methoxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-9-[[(2S,3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-1-oxo-4-hexenyl]oxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-(1-oxopropoxy)-7,11-methano-

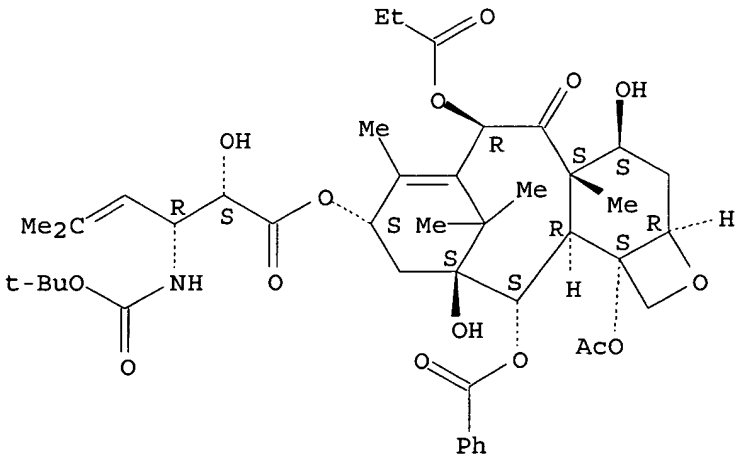
Rutter, Jessica; Ojima, Iwao
CORPORATE SOURCE: Department of Chemistry, State University of New York at Stony Brook, Stony Brook, NY, 11794-3400, USA
SOURCE: Chirality (2000), 12(5/6), 431-441
CODEN: CHRLEP; ISSN: 0899-0042
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:150742

AB A series of highly potent second-generation taxoids bearing a 2-methylprop-1-enyl or a 2-methylpropyl group at C-3' with modifications at the C-2, C-10, and C-14 positions was synthesized through the coupling of racemic cis-β-lactams with properly protected/modified baccatin and 14-OH-baccatin. A high level of kinetic resolution was observed for all cases examined The observed highly efficient enantiomer differentiation is ascribed to the markedly different chiral environment between the (+)- and (-)-β-lactams in their approach to the chiral framework of the enantiopure lithium alkoxide of a baccatin in the ring-opening coupling process. It was also observed that substantially higher selectivity was achieved when 14-OH-baccatin-1,14-carbonate was used. Anal. of the transition state models revealed that the repulsive interactions between the 3-TIPS group of a (-)-β-lactam with 1,14-carbonate group of the baccatin substantially increases the asym. bias in the kinetic resolution process, favoring the reaction of a (+)-β-lactam, which leads to the observed excellent selectivity.

IT **287180-33-0P 287180-34-1P 287180-35-2P**
287180-36-3P 287180-37-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of highly potent second-generation taxoids through effective kinetic resolution coupling of racemic β-lactams with baccatins)

RN 287180-33-0 CAPLUS
CN 4-Hexenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3R)- (9CI) (CA INDEX NAME)

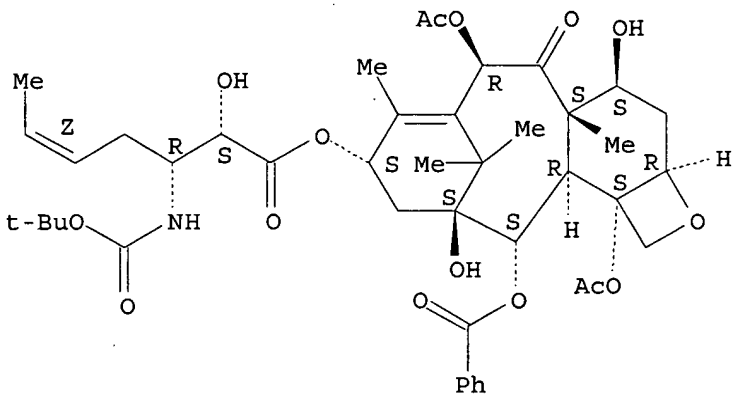
Absolute stereochemistry.



RN 287180-34-1 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-

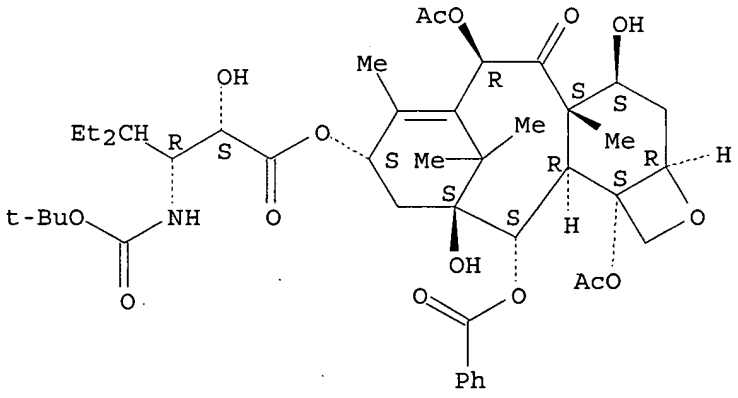
(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3R,5Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 292608-64-1 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4-ethyl-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



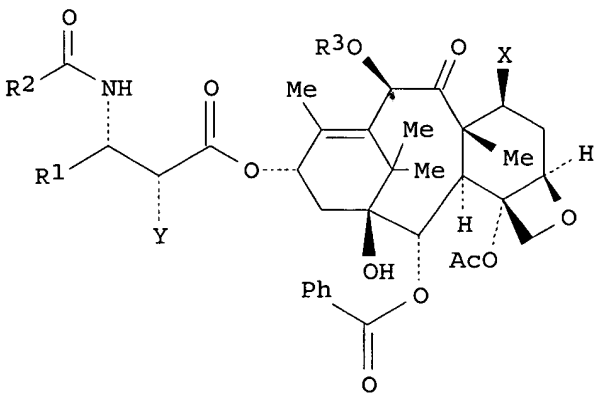
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 20 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:374253 CAPLUS
DOCUMENT NUMBER: 133:150742
TITLE: Synthesis of highly potent second-generation taxoids through effective kinetic resolution coupling of racemic β-lactams with baccatins
AUTHOR(S): Lin, Songnian; Geng, Xudong; Qu, Chuanxing; Tynebor, Robert; Gallagher, David J.; Pollina, Elizabeth;

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000053592	A1	20000914	WO 2000-JP1334	20000306
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2003026673	A2	20030129	JP 1999-59415	19990305
PRIORITY APPLN. INFO.:			JP 1999-59415 A	19990305
OTHER SOURCE(S):	MARPAT 133:238151			

GI



I

AB Claimed are osteogenesis promoters containing taxoids represented by general formula (I) in amts. effective for osteogenesis (wherein X and Y are each independently hydroxyl or a group convertible into hydroxyl in vivo; R1 is alkyl, alkenyl, alkynyl, Ph, naphthyl, furyl, or thienyl; R2 is alkyl, Ph, naphthyl, furyl, thienyl, alkoxy, or alkylamino; and R3 is hydrogen, alkyl, alkylcarbonyl, benzoyl, naphthoyl, furoyl, thenoyl, alkoxycarbonyl, or dialkylcarbamoyl) for the treatment of bone fracture and bone loss due to surgical bone removal. Thus, de-N-benzoyl-3'-desphenyl-3'-isobutylpaclitaxel (preparation given) was acylated by di-tert-amyl dicarbonate in a mixture of EtOAc and saturated aqueous NaHCO3 at room temperature for 5 h to give de-N-benzoyl-N-tert-amyloxycarbonyl-3'-desphenyl-3'-isobutylpaclitaxel (II). II in vitro increased number of bone nodules formed in rat osteoblastic cell from 5.3±5.2 (control) to 25, 64, and 97/well at 0.3, 1, and 4 ng/mL, resp.

IT **292608-56-1P 292608-64-1P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of taxoid compds. as osteogenesis promoters for treatment of bone fracture and bone loss due to surgical bone removal)

RN 292608-56-1 CAPLUS

CN 5-Heptenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-,

Miao, Fang-ming
CORPORATE SOURCE: School of Chemical Engineering, Tianjin University, Tianjin, 300072, Peop. Rep. China
SOURCE: Tianjin Daxue Xuebao, Ziran Kexue Yu Gongcheng Jishuban (2000), 33(1), 51-55
CODEN: TDXZAE
PUBLISHER: Tianjin Daxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

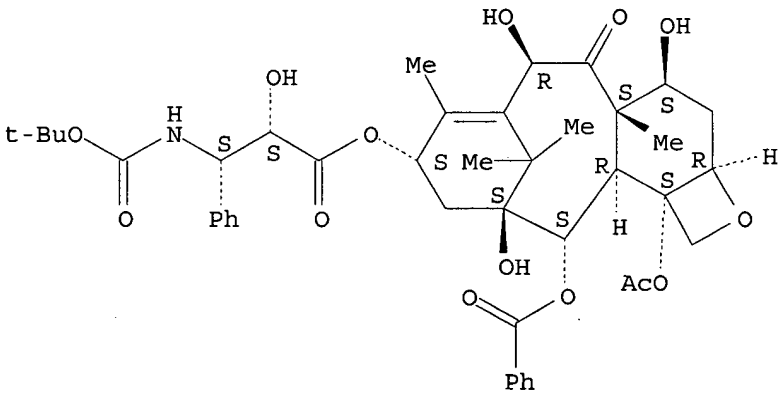
AB A series of 58 paclitaxel analogs with different pharmacophores have been investigated using the comparative mol. field anal. (CoMFA), and a 3D-quant. structure-activity relationship (3D-QSAR) model with high prediction has been obtained. The model is very significant for the research and development of novel paclitaxel analogs and decreasing the blindness in drug design.

IT **133577-33-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(development and application of 3D-quant. structure-activity relationship model of paclitaxel analogs)

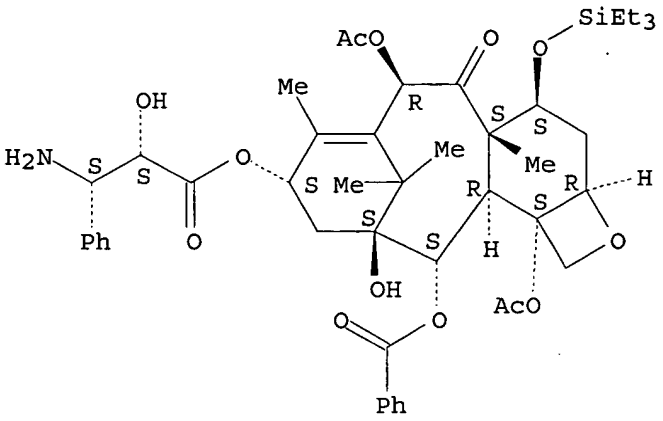
RN 133577-33-0 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

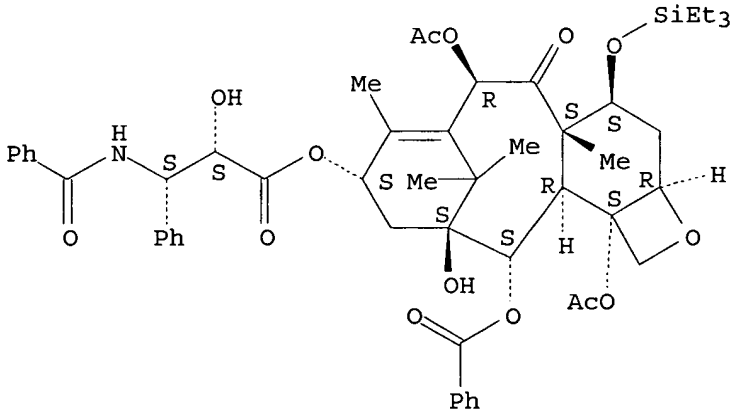


L51 ANSWER 19 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:646001 CAPLUS
DOCUMENT NUMBER: 133:238151
TITLE: Preparation of taxoid compounds as osteogenesis promoters
INVENTOR(S): Ishizuya, Toshinori; Ikuta, Shunichi; Uzawa, Toyonobu; Hori, Masayuki
PATENT ASSIGNEE(S): Asahi Kasei Kogyo Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 152 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1



IT **301835-15-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of taxoid compds.)
RN 301835-15-4 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

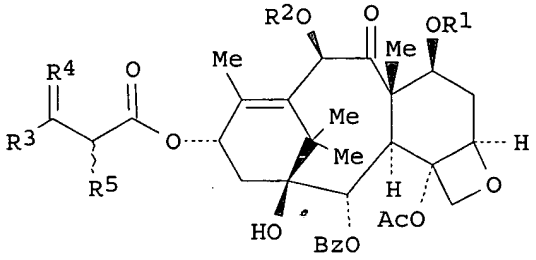
Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 18 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:704912 CAPLUS
DOCUMENT NUMBER: 134:187814
TITLE: Development and application of 3D-quantitative structure-activity relationship model of paclitaxel analogs
AUTHOR(S): Liu, Bin; Shi, Bing-xing; Yuan, Ying-jin; Sun, Ming;

IE, SI, LT, LV, FI, RO
PRIORITY APPLN. INFO.: JP 1999-263974 A 19990917
OTHER SOURCE(S): MARPAT 133:310031
GI



I

AB A method for the preparation of taxoid compds. (I) [R1, R2 = hydroxy protecting group; R3 = aryl, heteroaryl, alkyl, hydroxyalkyl, haloalkyl, cycloalkyl etc.; R4 = NOR6 ; R5 = OH; R6 = CH2Ph, Me, Et, COPh, COMe] was developed. Thus, I [R1 = TES, R2 = BOC, R3 = Ph, R4 = N-OBn, R5 = α-OH (II)] was prepared by oximation with O-benzylhydroxylamine hydrochloride of protected 10-deacetylbaccatin III, followed by azotization with tosyl azide, reaction with copper acetylacetonate and deacetylation of acetoxyoxime in presence of 1-chloro-3-hydroxytetrabutylsiloxane. Methods for producing the taxoid derivative I (R4 = O) from a baccatin derivative and other taxoid compds. such as paclitaxel from I (R4 = O) through intermediate compds. (amino-alc., benzoylamino-alc. and oxazoline) are also disclosed.

IT **301835-14-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of taxoid compds.)

RN 301835-14-3 CAPLUS

CN Benzenepropanoic acid, β-amino-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

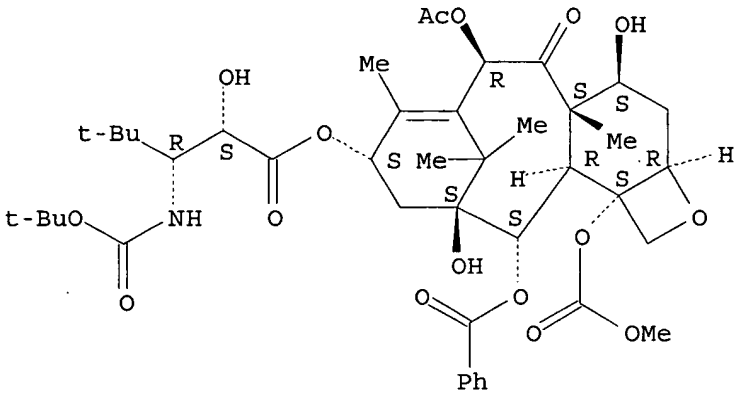
and paclitaxel (III) simultaneously or when III preceded II·HCl.

IT **364357-78-8P**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synergistic methods using two or more anticancer agents for treating cancer)

RN 364357-78-8 CAPLUS

CN D-threo-Pentonic acid, 3,4,5-trideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4-dimethyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-12b-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 17 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:752143 CAPLUS

DOCUMENT NUMBER: 133:310031

TITLE: methods for preparation of taxoid compounds from baccatin derivatives

INVENTOR(S): Mandai, Tadakatsu; Okumoto, Hiroshi; Nakanishi, Katsuyoshi; Hara, Koji; Mikuni, Katsuhiko; Hara, Kozo

PATENT ASSIGNEE(S): Bio Research Corporation of Yokohama, Japan; Ensuiko Sugar Refining Co., Ltd.

SOURCE: U.S., 19 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6136990	A	20001024	US 2000-504788	20000215
JP 2001089464	A2	20010403	JP 1999-263974	19990917
AU 724835	B1	20000928	AU 2000-17557	20000217
CA 2299967	AA	20010317	CA 2000-2299967	20000229
CA 2299967	C	20050419		
EP 1085018	A1	20010321	EP 2000-103473	20000301

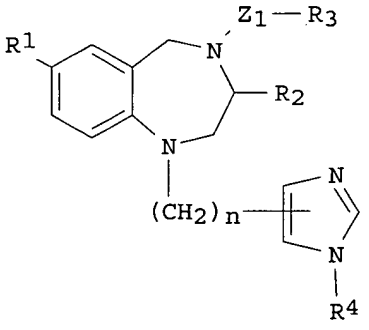
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

PATENT INFORMATION:

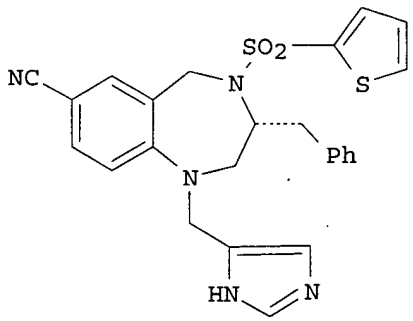
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001072721	A2	20011004	WO 2001-US9193	20010322
WO 2001072721	A3	20020613		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2404712	AA	20011004	CA 2001-2404712	20010322
EP 1272193	A2	20030108	EP 2001-920653	20010322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003528864	T2	20030930	JP 2001-570634	20010322
RU 2264217	C2	20051120	RU 2002-129000	20010322
BR 2001009517	A	20060829	BR 2001-9517	20010322
US 2002002162	A1	20020103	US 2001-817456	20010326
US 6537988	B2	20030325		
NO 2002004610	A	20021125	NO 2002-4610	20020926
ZA 2002007766	A	20030120	ZA 2002-7766	20020926
PRIORITY APPLN. INFO.:			US 2000-192278P P	20000327
			WO 2001-US9193 W	20010322

OTHER SOURCE(S): MARPAT 135:288636

GI



I



II

AB The present invention provides a synergistic method for the treatment of cancer which comprises administering a synergistically, therapeutically effective amount of: (i) at least agent selected from the group consisting of cytotoxic agents and cytostatic agents, and (ii) a compound of formula [I; R1 = Cl, Br, CN, substituted Ph, substituted pyridyl; R2 = alkyl, aralkyl; R3,R5 = substituted alkyl, aryl, heterocycle; R4 = H, alkyl; Z1 = CO, SO2, CO2, SO2N(R5); n = 1,2] or a pharmaceutically acceptable salt thereof. The present invention further provides a pharmaceutical composition for the synergistic treatment of cancer which comprises at least one agent selected from the group consisting of antiproliferative cytotoxic agents and antiproliferative cytostatic agents, a compound of formula I, and a pharmaceutically acceptable carrier. Synergism was observed when non-proliferating tumor cells were treated with diazepine II·HCl

(3), 97-102
CODEN: HSDZER; ISSN: 1000-5463
PUBLISHER: Huanan Shifan Daxue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

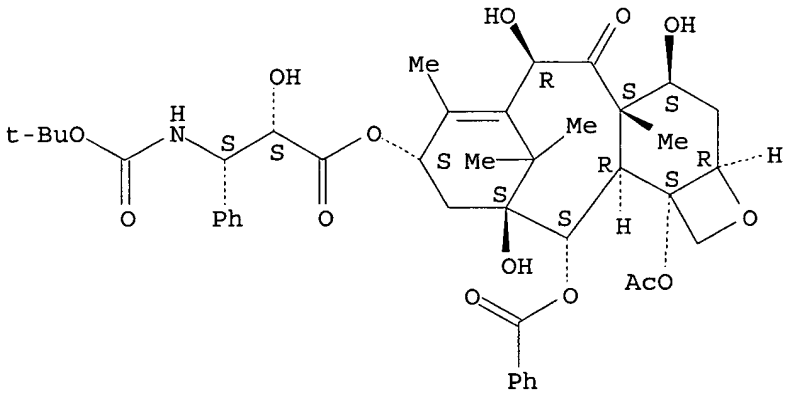
AB To analyze the QSAR of 13 paclitaxel analogs (for R6 = H), the MM3 geometry optimization and MNDO quantum chemical indexes have been performed. It is concluded that the change of R2 group, the sum of net charge of carbon and oxygen atoms of Bz in 2-O Bz Σ Q Bz, and the energy of core-core interaction Ep, affect the activity significantly. A significant quant. relationship between electronic structure and antimitotic activity of paclitaxel analogs was obtained as follows: ID50(A)/ID50(T)(act) = 71.20535+155.35016 Σ QBz. The QSAR reveals that the values of ID50(A)/ID50(T)(act) are decreased, and the activities are increased as the decrease of Σ Q Bz. The superior predictions were obtained, by neural network in the research.

IT **133577-33-0**
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(study on the relationships between the electronic structure and antimitotic activity of paclitaxel analogs)

RN 133577-33-0 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

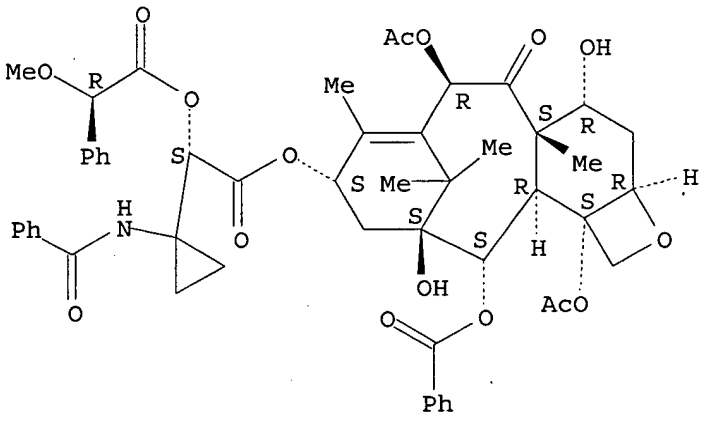
Absolute stereochemistry.



L51 ANSWER 16 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:730715 CAPLUS
DOCUMENT NUMBER: 135:288636
TITLE: Synergistic methods and compositions for treating cancer using two or more anticancer agents
INVENTOR(S): Lee, Francis Y.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

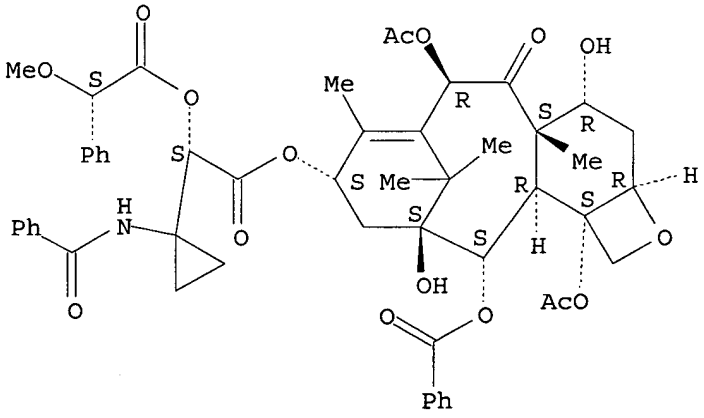
9-yl]oxy]-2-oxoethyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 534572-30-0 CAPLUS
CN Benzeneacetic acid, α-methoxy-, (1S)-1-[1-(benzoylamino)cyclopropyl]-2-[[(2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl]oxy]-2-oxoethyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

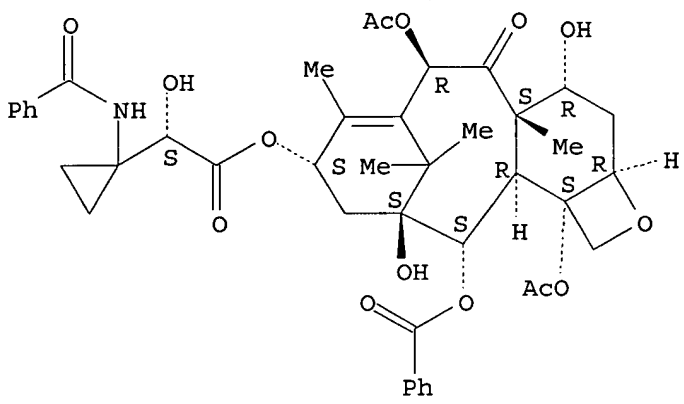


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 15 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:824014 CAPLUS
DOCUMENT NUMBER: 137:27784
TITLE: Study on the relationships between the electronic structure and antimitotic activity of paclitaxel analogs. (I)
AUTHOR(S): Xu, Zhi-guang; Xu, Xuan; Luo, Yi-fan; Li, Wei-hua
CORPORATE SOURCE: Dep. Chem., South China Normal Univ., Canton, 510631, Peop. Rep. China
SOURCE: Huanan Shifan Daxue Xuebao, Ziran Kexueban (2001),

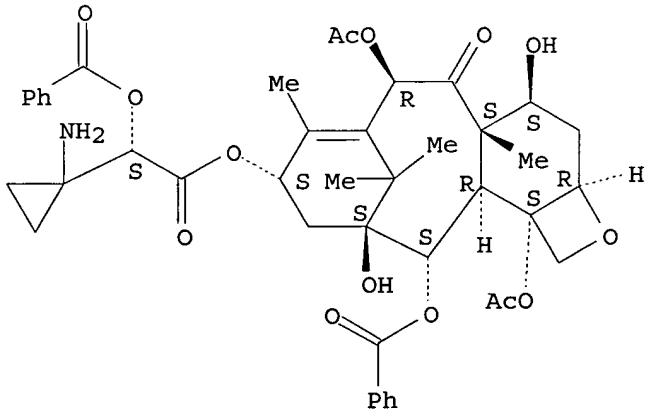
ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



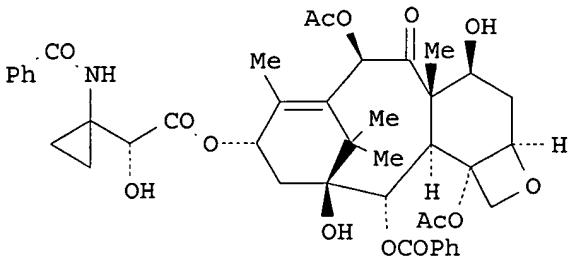
IT **534572-19-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and anti-cancer activity of paclitaxel analogs with a cyclopropanated side-chain)
RN 534572-19-5 CAPLUS
CN Cyclopropaneacetic acid, 1-amino-α-(benzoyloxy)-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

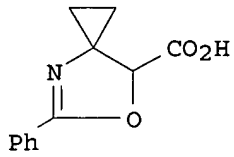


IT **534572-29-7P 534572-30-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and anti-cancer activity of paclitaxel analogs with a cyclopropanated side-chain)
RN 534572-29-7 CAPLUS
CN Benzeneacetic acid, α-methoxy-, (1S)-1-[1-(benzoylamino)cyclopropyl]-2-[[(2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-

LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:7034
GI



I



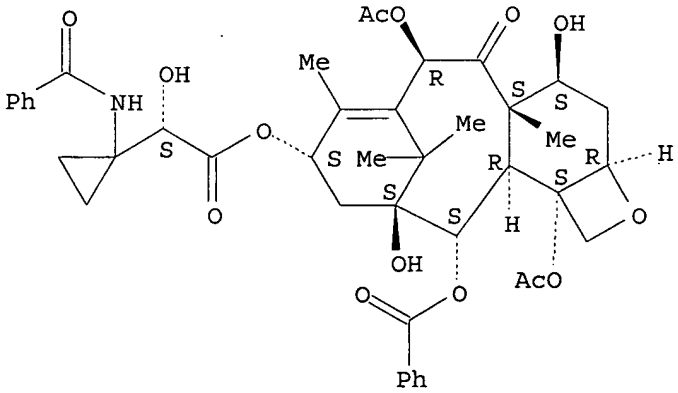
II

AB Four paclitaxel analogs, such as I, with a cyclopropanated side-chain were synthesized by coupling of the spirocyclopropanated oxazoline-5-carboxylic acid II with 7-O-(triethylsilyl)baccatin III, followed by hydrolytic ring opening and rearrangement. The absolute configuration of the 2'-position was determined by NMR anal. of the corresponding Mosher esters. The two new paclitaxel analogs with the R configuration at C-2' were both active in the A2780 mammalian cell line cytotoxicity assay, but much less than paclitaxel itself.

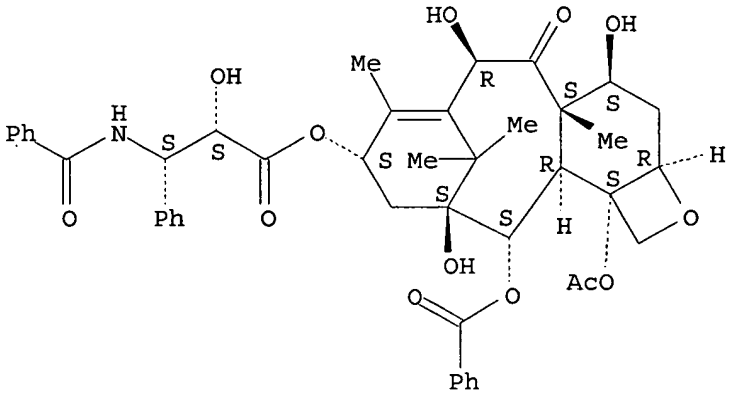
IT **534572-23-1P 534572-25-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and anti-cancer activity of paclitaxel analogs with a cyclopropanated side-chain)

RN 534572-23-1 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

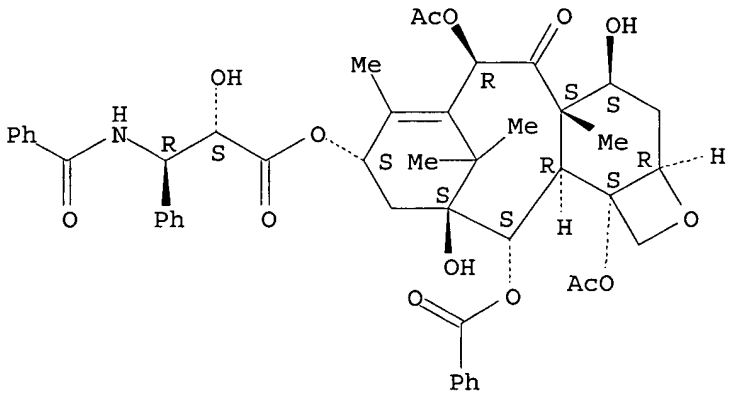


RN 534572-25-3 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl



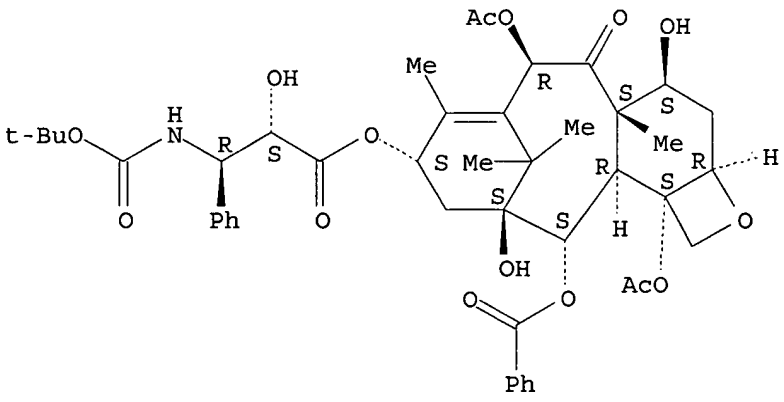
RN 149197-23-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



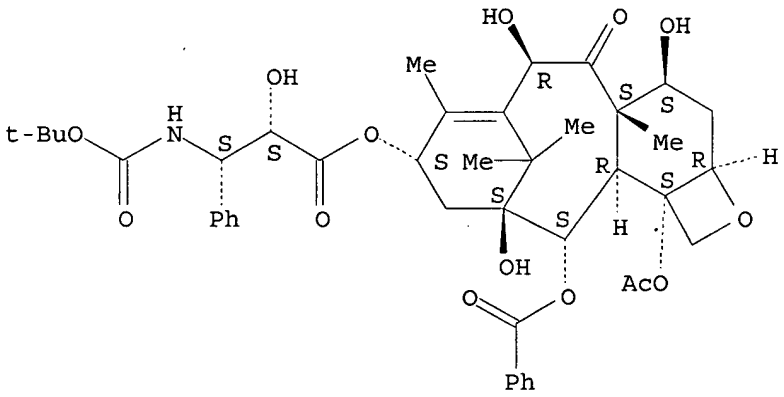
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 14 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:128638 CAPLUS
DOCUMENT NUMBER: 139:7034
TITLE: Synthesis and bioactivities of paclitaxel analogs with a cyclopropanated side-chain
AUTHOR(S): Liu, Changhui; Tamm, Markus; Notzel, Marcus W.; de Meijere, Armin; Schilling, Jennifer K.; Kingston, David G. I.
CORPORATE SOURCE: Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061, USA
SOURCE: Tetrahedron Letters (2003), 44(10), 2049-2052 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal



RN 133577-33-0 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

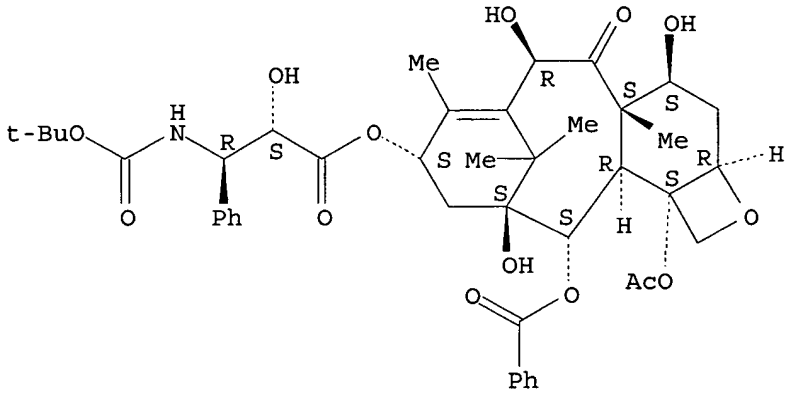


RN 133577-35-2 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

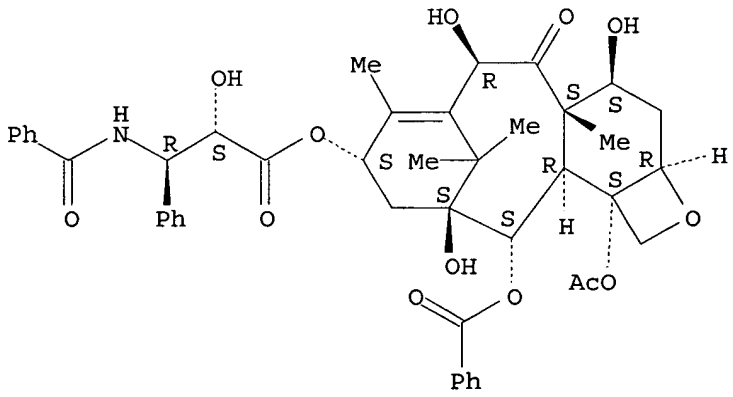
α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 125354-13-4 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

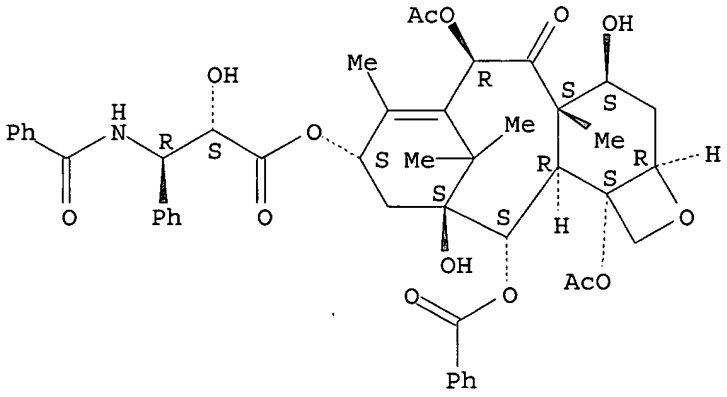
Absolute stereochemistry.



RN 125354-17-8 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.



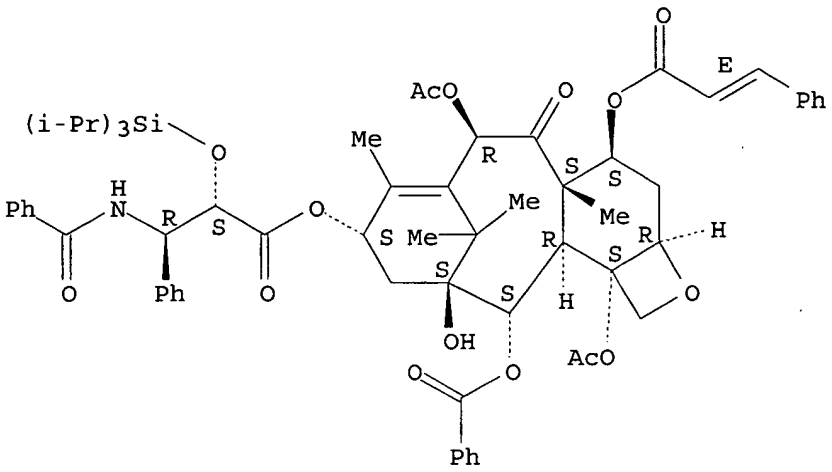
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 13 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:151052 CAPLUS
DOCUMENT NUMBER: 138:331208
TITLE: A Structure-Activity Study of Taxol, Taxotere, and Derivatives Using the Electronic Indices Methodology (EIM)
AUTHOR(S): Braga, S. F.; Galvao, D. S.
CORPORATE SOURCE: Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, Campinas, 13083-970, Brazil
SOURCE: Journal of Chemical Information and Computer Sciences (2003), 43(2), 699-706
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Among the new families of effective anticancer drugs, the natural product paclitaxel (Taxol/Bristol-Myers-Squibb) and its semisynthetic derivative docetaxel (Taxotere/Rhone-Poulenc Rorer) are probably the most promising agents under investigation. Surprisingly considering their importance no detailed quantum mech. studies have been carried out for these drugs. In this work we report the first structure-activity relation (SAR) studies for 20 taxoid structures using mol. descriptors from all-electron quantum methods. The used methods were the pattern-recognition Principal Component Anal. (PCA), Hierarchical Clustering Anal. (HCA), and the recently developed Electronic Indexes Methodol. (EIM). The combined use of EIM with PCA/HCA methodologies was able to correctly classify active and inactive taxoids with 100% of accuracy using only a few "universal" quantum mol. descriptors. It was possible to identify the electronic features defining active mols. This information can be used to select and design new active compds. The combined use of EIM with PCA/HCA can be a new and very efficient tool in the field of computer assisted drug design.

IT **114977-29-6 125354-13-4 125354-17-8 133577-33-0 133577-35-2 149197-23-9**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity study of Taxol, Taxotere, and derivs. using the electronic indexes methodol.)

RN 114977-29-6 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

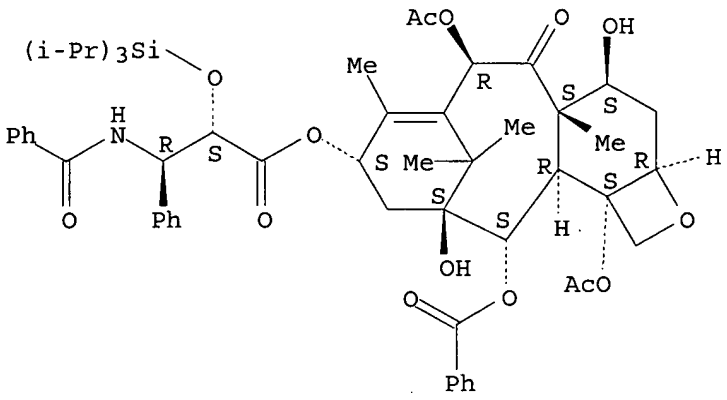
L51 ANSWER 12 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:326401 CAPLUS
DOCUMENT NUMBER: 140:35302
TITLE: 3D QSAR studies of the interaction between β-tubulin and microtubule stabilizing antimitotic agents (MSAA). A combined pharmacophore generation and pseudoreceptor modeling approach applied to taxanes and epothilones
AUTHOR(S): Manetti, Fabrizio; Forli, Stefano; Maccari, Laura; Corelli, Federico; Botta, Maurizio
CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico, Universita degli Studi di Siena, Siena, I-53100, Italy
SOURCE: Farmaco (2003), 58(5), 357-361
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Based on the conformer of paclitaxel extracted from the exptl. tubulin structure, a pharmacophoric model has been generated and used to find the chemical features common to the taxane and epothilone classes of compds. This original alignment has been translated into the exptl. tubulin binding site obtaining an assembly subsequently submitted to the pseudoreceptor modeling approach. As a result, an original 3D QSAR model, able to evaluate, at a quant. level, the relationships between the mol. structures and biol. data of the studied compds., has been obtained.

IT **149197-23-9**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of the interaction between β-tubulin and microtubule stabilizing antimitotic agents)

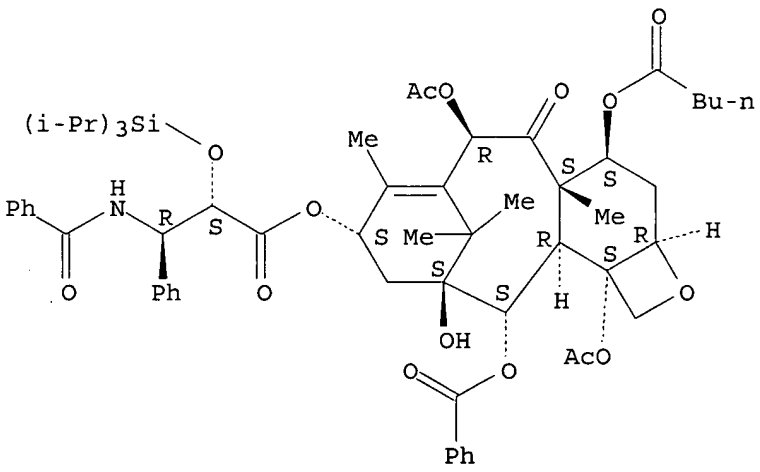
RN 149197-23-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



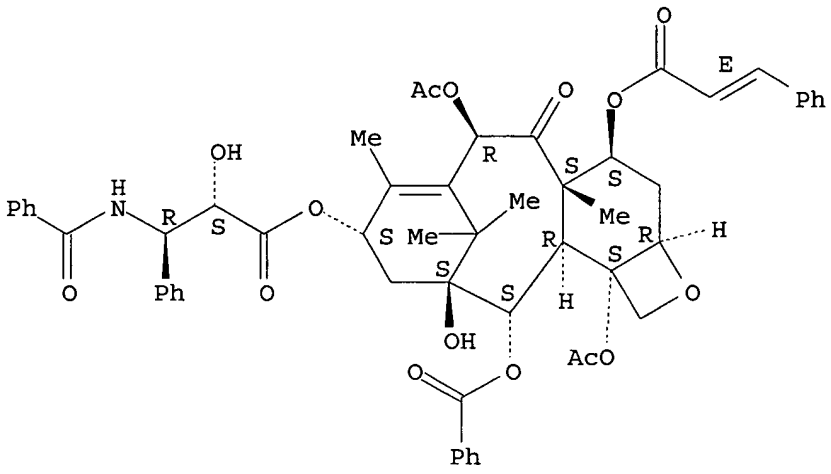
RN 618428-51-6 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-[[tris(1-methylethyl)silyl]oxy]-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(1-oxopentyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 618428-65-2 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-[[tris(1-methylethyl)silyl]oxy]-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

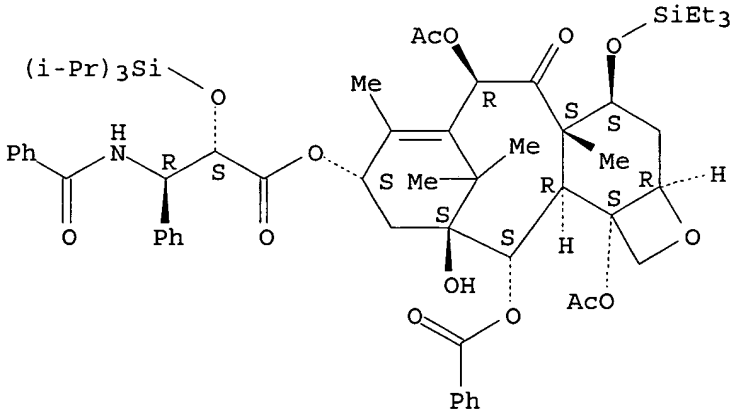
Absolute stereochemistry.
Double bond geometry as shown.



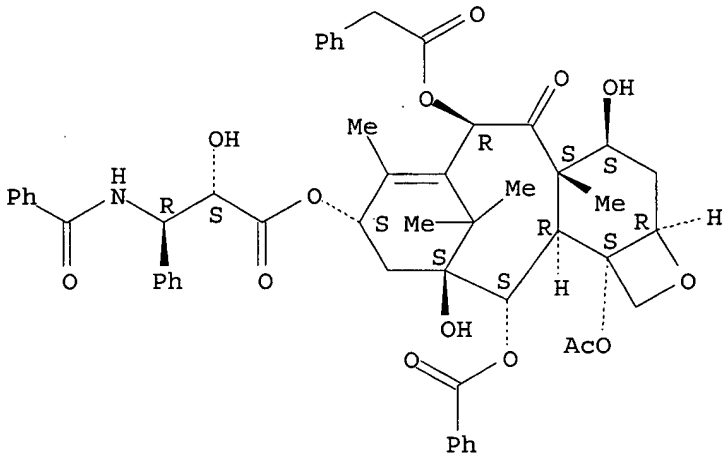
IT **618428-04-9P 618428-05-0P 618428-51-6P 618428-65-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of taxoids and their ability to activate murine macrophages and inhibition of the growth of macrophage-like cells)

RN 618428-04-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-[[tris(1-methylethyl)silyl]oxy]-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

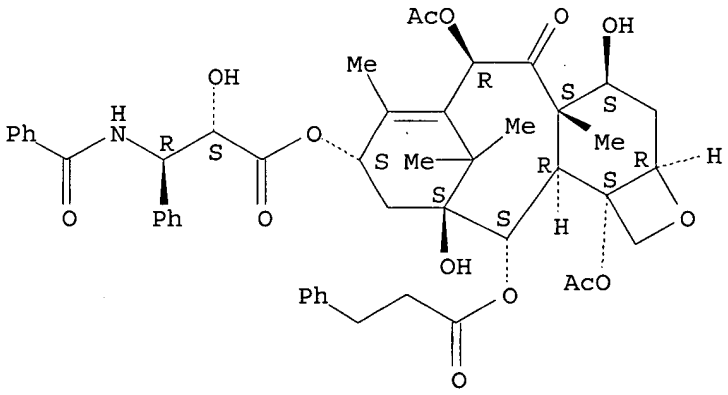


RN 618428-05-0 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-[[tris(1-methylethyl)silyl]oxy]-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)



RN 618428-39-0 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12-(1-oxo-3-phenylpropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

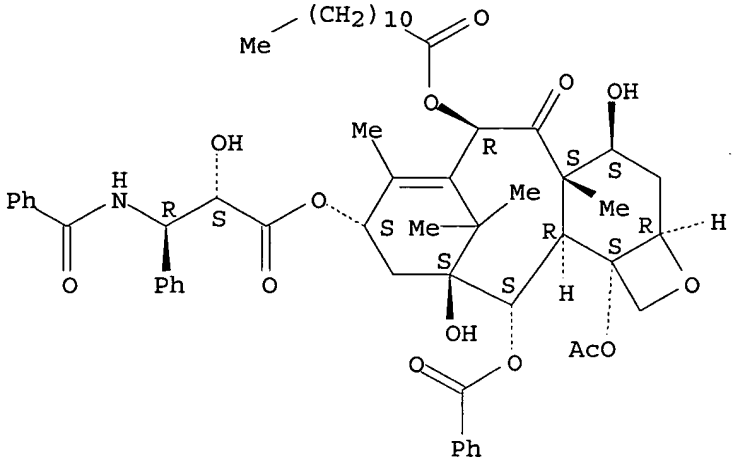
Absolute stereochemistry.



RN 618428-55-0 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

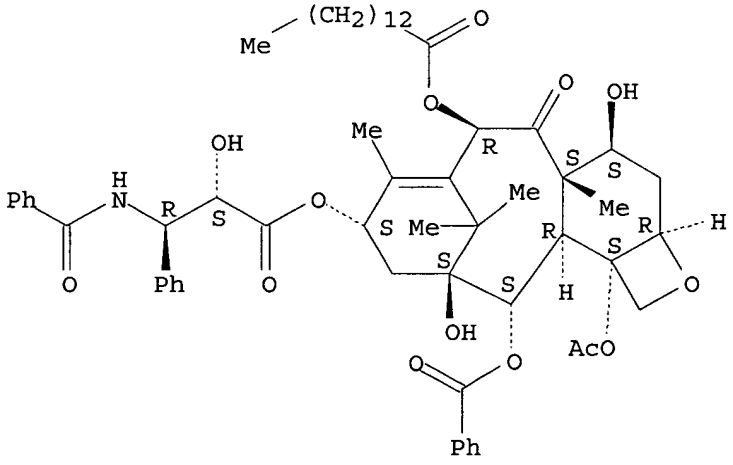
Absolute stereochemistry.
Double bond geometry as shown.

Absolute stereochemistry.



RN 618428-14-1 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-[(1-oxotetradecyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

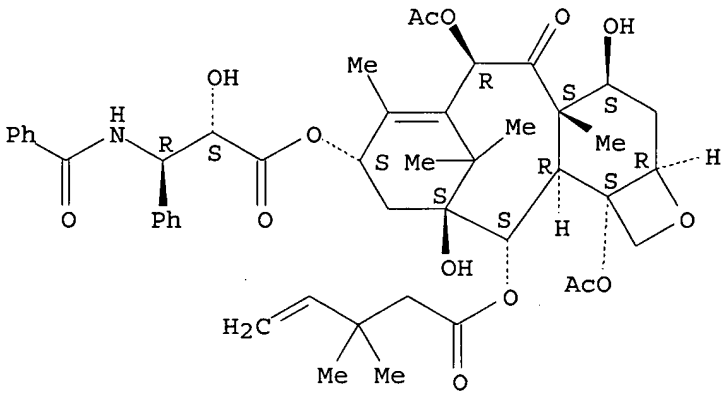
Absolute stereochemistry.



RN 618428-15-2 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-[(phenylacetyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

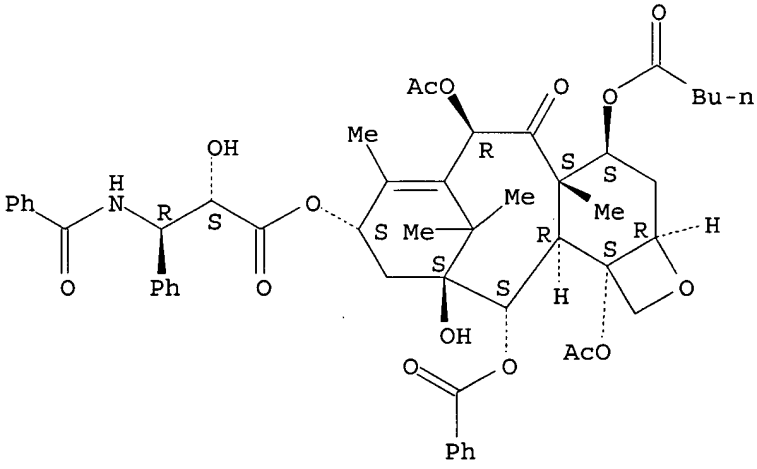


IT **618428-06-1P 618428-13-0P 618428-14-1P**
618428-15-2P 618428-39-0P 618428-55-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of taxoids and their ability to activate murine macrophages and inhibition of the growth of macrophage-like cells)

RN 618428-06-1 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(1-oxopentyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 618428-13-0 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-[(1-oxododecyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

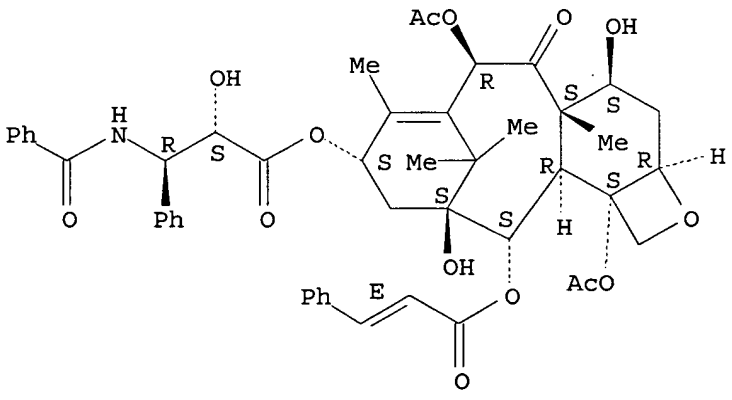
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:350856

AB A series of new taxoids modified at the C-3', C-3'N, C-10, C-2 and C-7 positions was designed, synthesized and evaluated for their potency to induce NO and TNF production by peritoneal murine macrophages (Mϕ) from LPS-responsive C3H/HeN and LPS-hyporesponsive C3H/HeJ strains and human blood cells, and for their ability to inhibit the growth of Mϕ-like cell lines J774.1 and J7.DEF3. The SAR-study showed that the nature of the substituents at these positions are critical for the induction of TNF and NO production by Mϕ. Positions C-3' and C-10 are the most flexible, and an intriguing effect of the length of the substituents at the C-10 position is observed for taxoids bearing a straight chain alkanoyl moiety. An aromatic group at the C-3'N and C-2 positions is required for the activity, while only hydroxyl or acetyl substituents seem to be tolerated at the C-7 position. The natural stereochem. in the C-13 isoserine side chain of the taxoids is an absolute requirement for macrophage activation. There is no correlation between the ability of the taxoids to induce TNF/NO production in C3H/HeN Mϕ and the cytotoxicity against Mϕ-like cells.

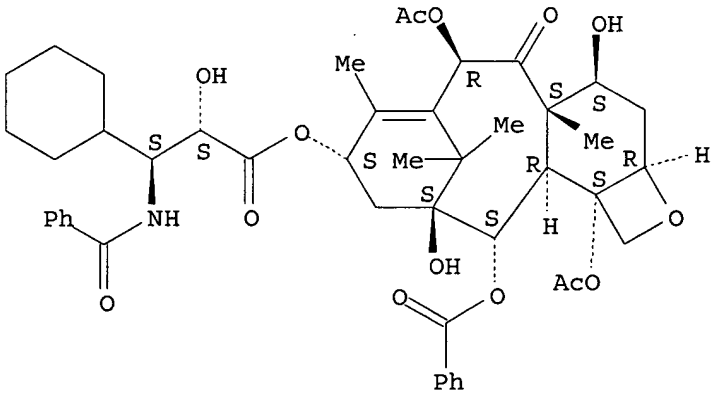
IT **618428-21-0P 618428-23-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of taxoids and their ability to activate murine macrophages and inhibition of the growth of macrophage-like cells)

RN 618428-21-0 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

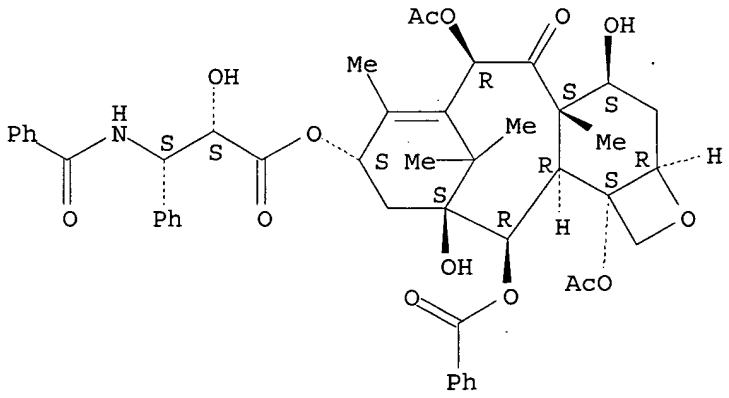


RN 618428-23-2 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-[(3,3-dimethyl-1-oxo-4-pentenyl)oxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)



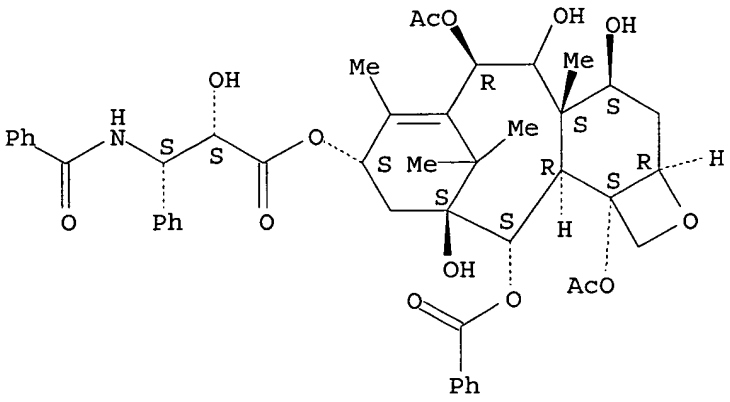
RN 676235-24-8 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12R,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



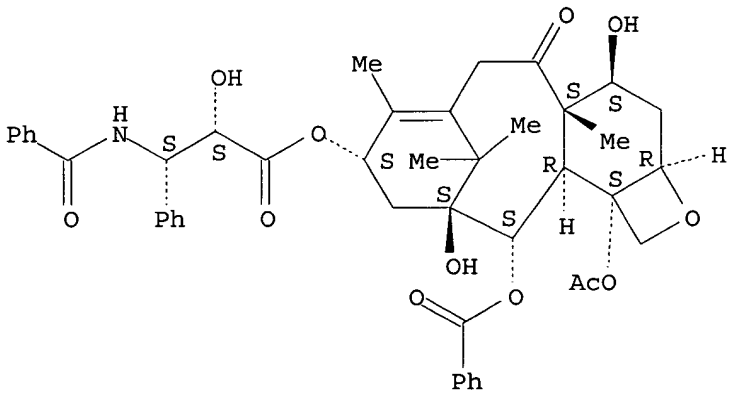
REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 11 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:427763 CAPLUS
DOCUMENT NUMBER: 139:350856
TITLE: Structure-activity relationship study of taxoids for their ability to activate murine macrophages as well as inhibit the growth of macrophage-like cells
AUTHOR(S): Ojima, Iwao; Fumero-Oderda, Cecilia L.; Kuduk, Scott D.; Ma, Zhuping; Kirikae, Fumiko; Kirikae, Teruo
CORPORATE SOURCE: Department of Chemistry, State University of New York at Stony Brook, Stony Brook, NY, 11794-3400, USA
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(13), 2867-2888
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal



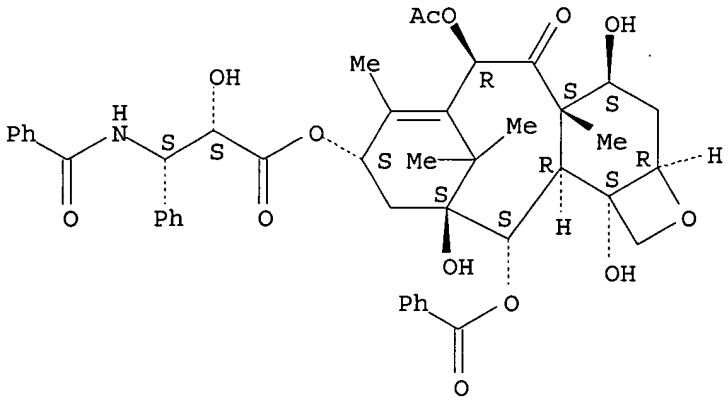
RN 675853-96-0 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



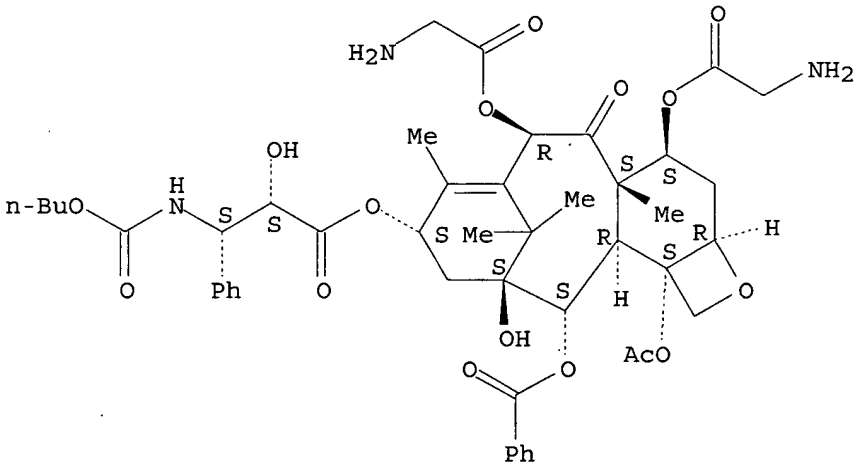
RN 675853-97-1 CAPLUS
CN Cyclohexanepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



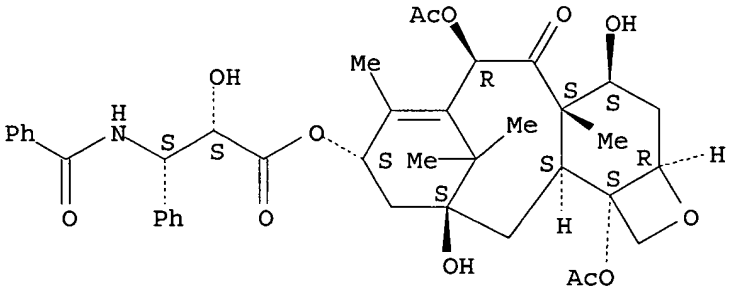
RN 675853-94-8 CAPLUS
CN Glycine, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-9-[(2S,3S)-3-[(butoxycarbonyl)amino]-2-hydroxy-1-oxo-3-phenylpropoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxete-4,6-diyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



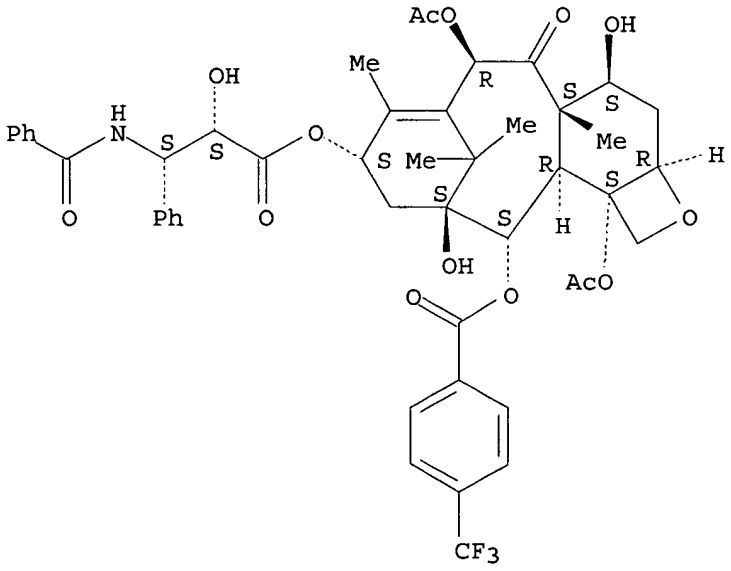
RN 675853-95-9 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,11-trihydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 675853-92-6 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-12-[[4-(trifluoromethyl)benzoyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

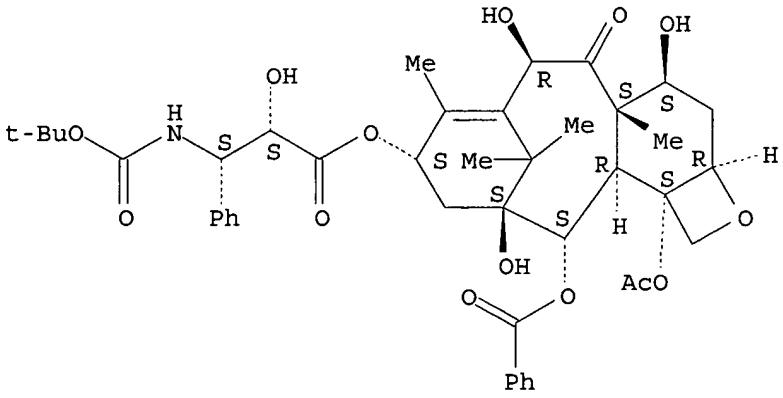
Absolute stereochemistry.



RN 675853-93-7 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11,12b-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

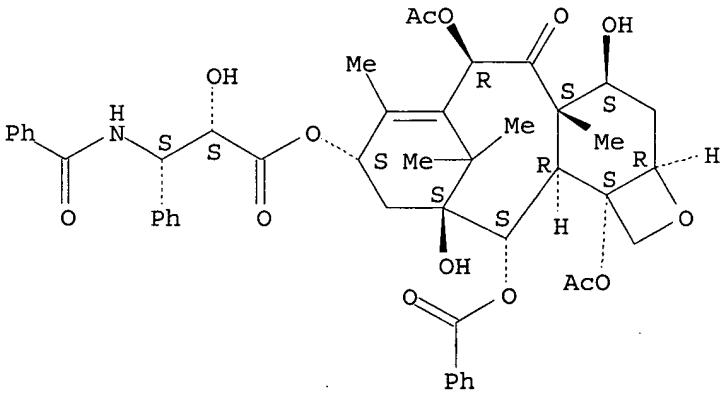
Absolute stereochemistry.

Absolute stereochemistry.



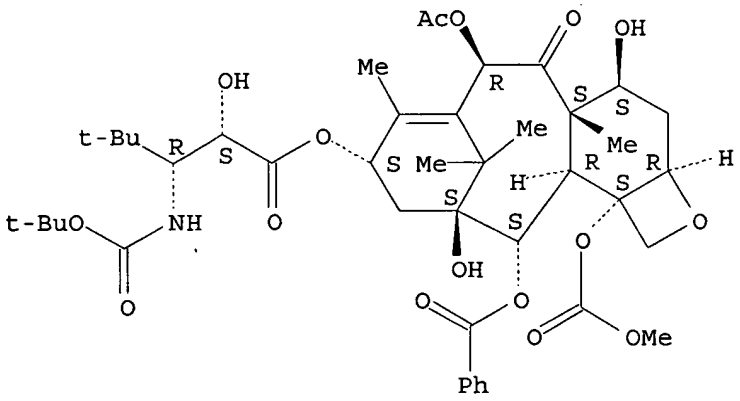
RN 179798-21-1 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 675853-91-5 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12aS,12bS)-6,12b-bis(acetyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



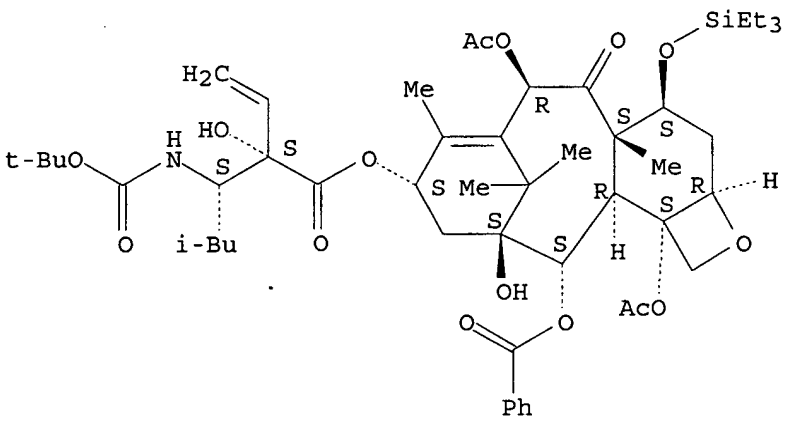
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 10 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:725913 CAPLUS
DOCUMENT NUMBER: 140:280729
TITLE: 3D QSAR studies for the β-tubulin binding site of microtubule-stabilizing anticancer agents (MSAAs). A pseudoreceptor model for taxanes based on the experimental structure of tubulin
AUTHOR(S): Maccari, Laura; Manetti, Fabrizio; Corelli, Federico; Botta, Maurizio
CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico, Universita degli Studi di Siena, Siena, I-53100, Italy
SOURCE: Farmaco (2003), 58(9), 659-668
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The antimitotic agent paclitaxel continues to play an important role in the cancer chemotherapy. However, its inefficacy on certain resistant cells and toxic side effects have led to the search of new taxanes with improved biol. activity. By a pseudoreceptor modeling approach, we have developed a binding site model for a series of taxanes. It is the first 3D QSAR model derived from the exptl. determined tubulin structure obtained by electron crystallog. studies. The model is able to correlate quant. the structural properties of the studied compds. with their biol. data.

IT **133577-33-0 179798-21-1 675853-91-5 675853-92-6 675853-93-7 675853-94-8 675853-95-9 675853-96-0 675853-97-1 676235-24-8**, 2,2'-epi-Taxol
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(3D QSAR studies for the β-tubulin binding site of microtubule-stabilizing anticancer agents (MSAAs). a pseudoreceptor model for taxanes based on the exptl. structure of tubulin)

RN 133577-33-0 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

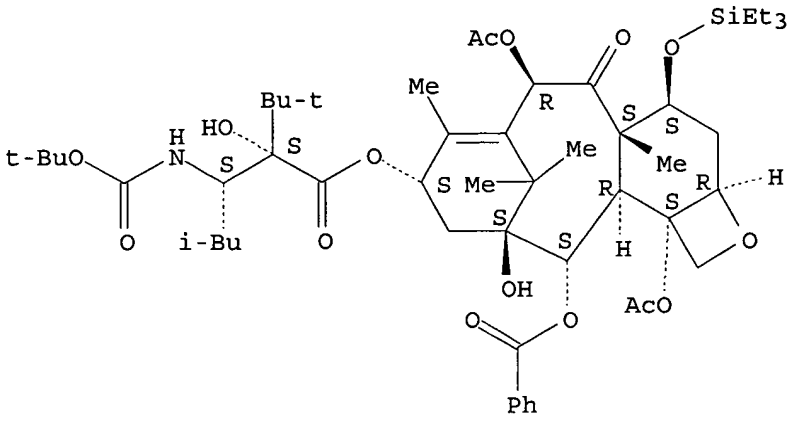
L51 ANSWER 9 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:728097 CAPLUS
DOCUMENT NUMBER: 140:192359
TITLE: The discovery of BMS-275183: an orally efficacious novel taxane
AUTHOR(S): Mastalerz, Harold; Cook, Donald; Fairchild, Craig R.; Hansel, Steven; Johnson, Walter; Kadow, John F.; Long, Byron H.; Rose, William C.; Tarrant, James; Wu, Mu-Jen; Xue, May Quifen; Zhang, Guifen; Zoeckler, Mary; Vyas, Dolatrai M.
CORPORATE SOURCE: Discovery Chemistry, Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492-7660, USA
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(20), 4315-4323
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:192359

AB The evolution of a C-4-methylcarbonate analog of paclitaxel with minimal oral bioavailability and oral efficacy, into its C-3'-t-butyl-3'-N-t-butyloxycarbonyl analog , a novel taxane with oral efficacy in preclin. models that is comparable to iv administered paclitaxel, is described.

IT **364357-78-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(discovery of BMS-275183, an orally efficacious novel taxane for cancer treatment)

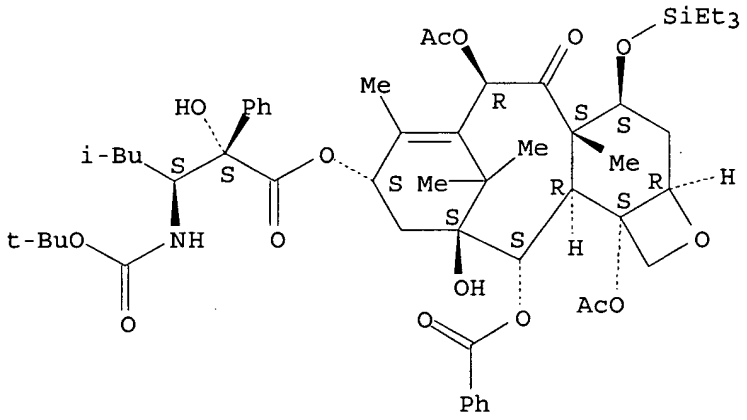
RN 364357-78-8 CAPLUS
CN D-threo-Pentonic acid, 3,4,5-trideoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4-dimethyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-12b-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 849829-72-7 CAPLUS
CN Benzeneacetic acid, α-[(1S)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methylbutyl]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

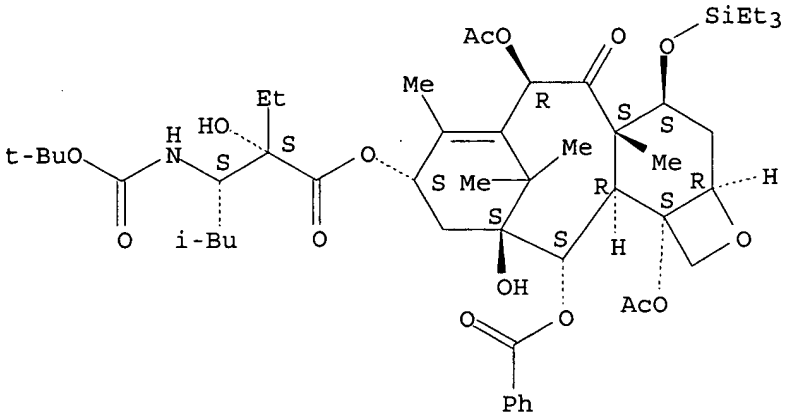


RN 849829-73-8 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-ethenyl-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

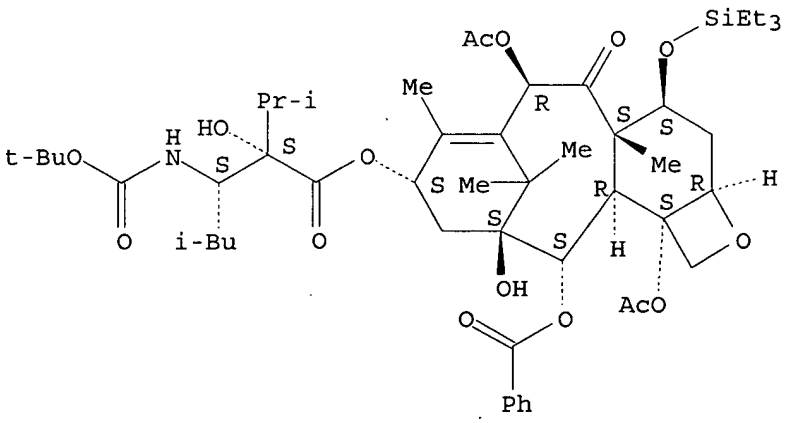
cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 849829-70-5 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-2-(1-methylethyl)-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 849829-71-6 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1,1-dimethylethyl)-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

2'-Substituted Taxanes as Probes for an Improved Protocol of Diastereomeric Differentiation

AUTHOR(S): Dambruoso, Paolo; Bassarello, Carla; Bifulco, Giuseppe; Appendino, Giovanni; Battaglia, Arturo; Fontana, Gabriele; Gomez-Paloma, Luigi

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Facolta di Farmacia, Universita di Salerno, Fisciano (SA), 84084, Italy

SOURCE: Organic Letters (2005), 7(6), 983-986
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:392542

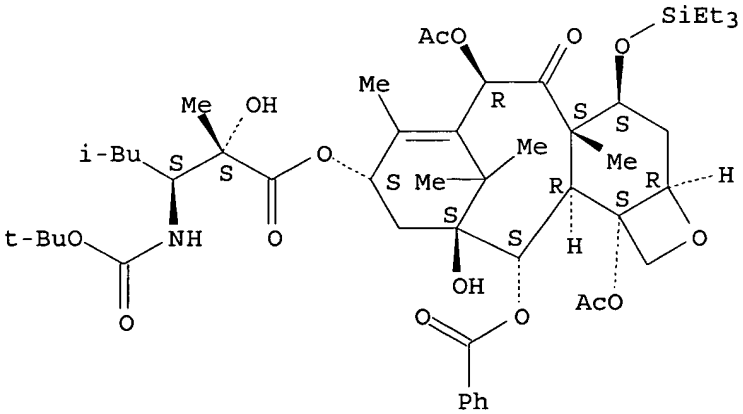
AB The configuration of the α-substituted α-hydroxy-β-aminoester moiety in a series of 2'-substituted taxanes was analyzed according to the recently proposed Universal NMR Database (UDB) approach. A critical anal. of the results showed that modifications regarding chemical shift adjustment (so as to render the shifts virtually connectivity independent) were necessary to get consistent stereo-assignments in this set of compds. On this basis, a modified UDB-based strategy, especially tailored to the configurational assignment of densely substituted diastereomeric fragments, is proposed.

IT **849829-68-1P 849829-69-2P 849829-70-5P**
849829-71-6P 849829-72-7P 849829-73-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and diastereomeric differentiation of α-substituted α-hydroxy-β-aminoester moiety in a series of 2'-substituted taxanes via universal NMR database approach)

RN 849829-68-1 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-2,5-dimethyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



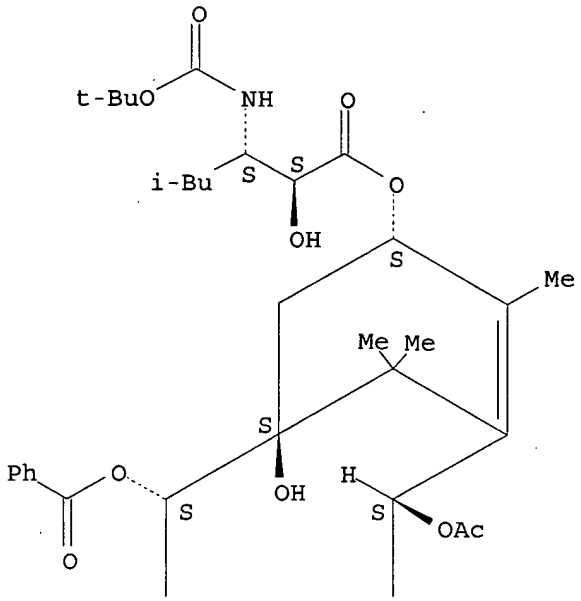
RN 849829-69-2 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-ethyl-2-hydroxy-5-methyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-

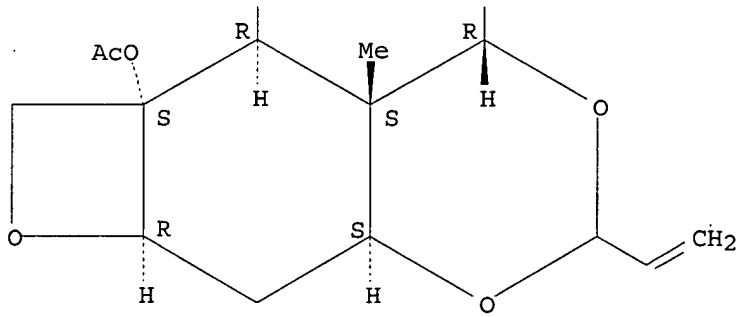
(Preparation)
(methods for the synthesis of 9,10-α,α-OH-taxane analogs)
RN 849213-17-8 CAPLUS
CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (1S,2S,4S,7S,7aR,10aS,11aR,13aS,13bR,13cS)-7,13a-bis(acetyloxy)-1-(benzoyloxy)-9-ethenyl-1,3,4,7,7a,10a,11,11a,13,13a,13b,13c-dodecahydro-2-hydroxy-5,13c,14,14-tetramethyl-2,6-methano-2H-cyclodec[de]oxeto[3,2-g][1,3]benzodioxin-4-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

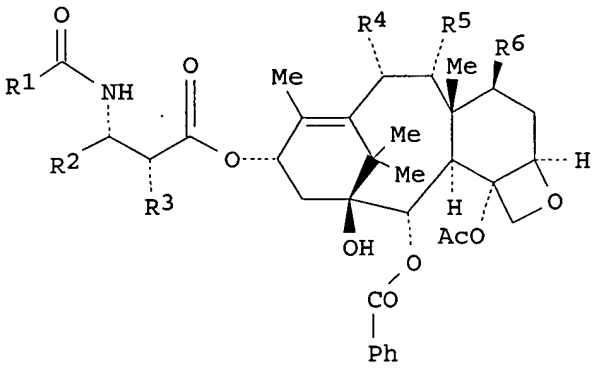
PAGE 1-A



PAGE 2-A



L51 ANSWER 8 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:134425 CAPLUS
DOCUMENT NUMBER: 142:392542
TITLE: Advances in the Universal NMR Database Approach.



I

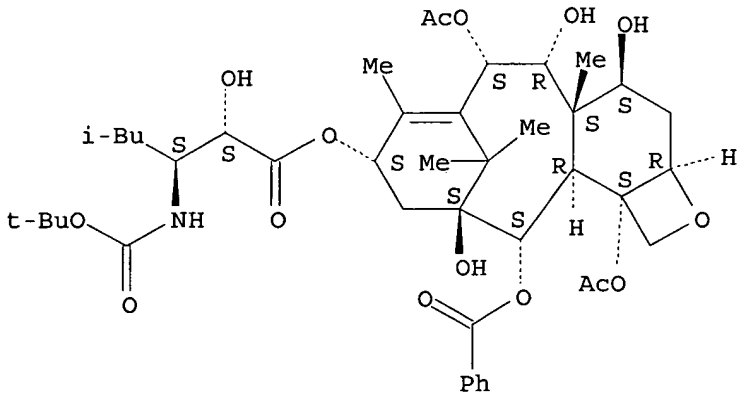
AB The present invention relates to new taxane analogs useful for the treatment of cancer as well as methods for producing the same. The chemical compds. according to the present invention have the general formula (I) wherein R1 and R2 are each selected from H, an alkyl group, an olefinic group, an aromatic group, an O-alkyl group, an O-olefinic group, or an O-aromatic group ; R3 is hydroxyl or OP1; R4 and R5 are each hydroxyl or R7COO ; R6 is hydroxyl, OP2, R7COO, or an ether functionality ; R7 is an alkyl group, an olefinic group, or an aromatic group ; and P1 and P2 are each hydroxyl protecting groups. The chemical compds. of the present invention may particularly be 9,10-α,α-OH taxane analogs that are formed by a process that begins with a standard taxane as the starting compound

IT **849213-16-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(methods for the synthesis of 9,10-α,α-OH-taxane analogs)

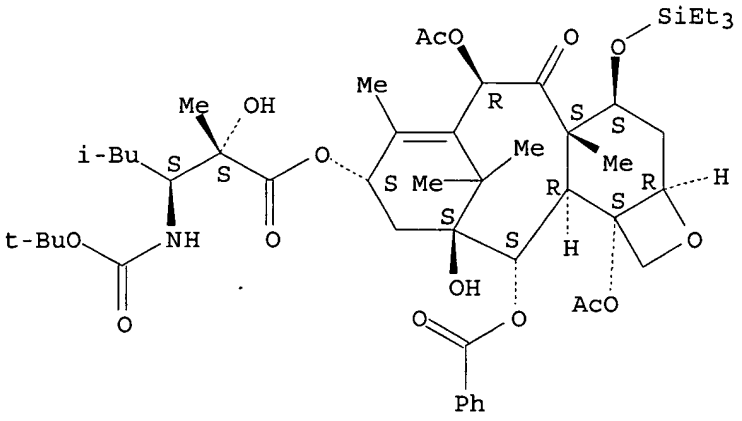
RN 849213-16-7 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-5-methyl-, (2aR,4S,4aS,5R,6S,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,5,11-trihydroxy-4a,8,13,13-tetramethyl-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **849213-17-8P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 7 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:300206 CAPLUS
DOCUMENT NUMBER: 142:373994
TITLE: Methods for the synthesis of 9,10-α,α-OH-taxane analogs
INVENTOR(S): McChesney, James D.; Ferrara, James; Zygmut, Jan
PATENT ASSIGNEE(S): Tapestry Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

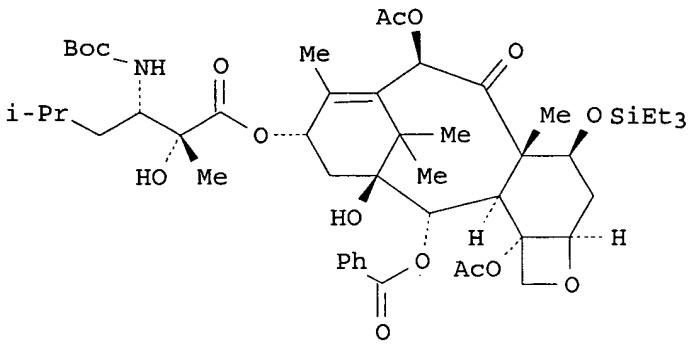
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030150	A2	20050407	WO 2004-US31816	20040927
WO 2005030150	A3	20050714		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004275881	A1	20050407	AU 2004-275881	20040927
CA 2539975	AA	20050407	CA 2004-2539975	20040927
US 2005148657	A1	20050707	US 2004-951555	20040927
EP 1664033	A2	20060607	EP 2004-789167	20040927
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				

PRIORITY APPLN. INFO.: US 2003-506680P P 20030925
WO 2004-US31816 W 20040927

OTHER SOURCE(S): MARPAT 142:373994
GI

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 6 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:336451 CAPLUS
DOCUMENT NUMBER: 143:26745
TITLE: 2'-Methyl taxanes: synthesis and NMR configurational assignment
AUTHOR(S): Dambruoso, Paolo; Bassarello, Carla; Bifulco, Giuseppe; Appendino, Giovanni; Battaglia, Arturo; Guerrini, Andrea; Fontana, Gabriele; Gomez-Paloma, Luigi
CORPORATE SOURCE: DISCAFF, Facolta di Farmacia, Universita del Piemonte Orientale, Largo Donegani, Novara, 2-28100, Italy
SOURCE: Tetrahedron Letters (2005), 46(19), 3411-3415
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:26745
GI



I

AB Capitalizing on an oxidation-alkylation approach, a non-diastereoselective entry into 2'-Me taxanes, e.g. I, was developed. The issue of configurational assignment at the newly formed side-chain quaternary stereocenter was solved and put into a more general context by integrating information from an alternative diastereoselective synthesis of model compds. and from spectroscopic measurements, critically comparing the J-Based and the Universal NMR Database approaches.

IT **849829-68-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and NMR configurational assignments of 2'-Me taxanes)

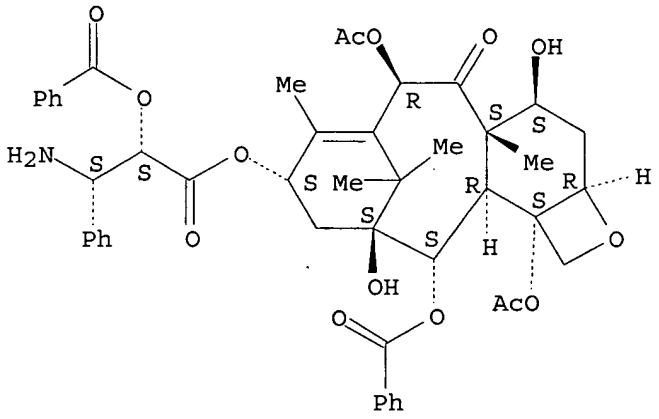
RN 849829-68-1 CAPLUS

CN Hexanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-2,5-dimethyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 179551-57-6 CAPLUS
CN Benzenepropanoic acid, β-amino-α-(benzoyloxy)-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, hydrochloride, (αS,βS)- (9CI) (CA INDEX NAME)

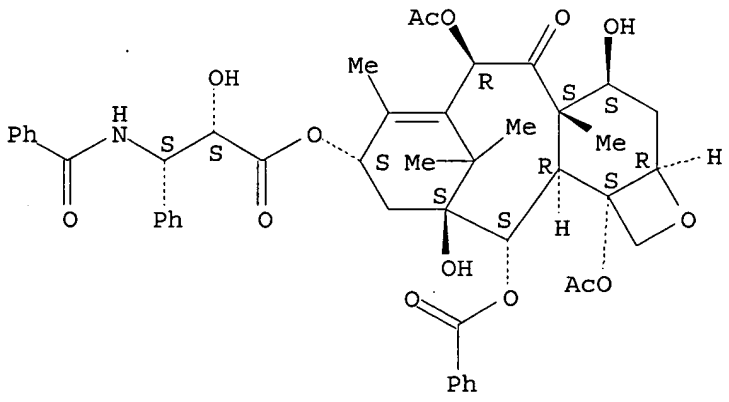
Absolute stereochemistry.



● HCl

IT **179798-21-1P**, 2'-epi-Paclitaxel
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation or C(2')-hydroxyl group inversion of; method for inverting the C(2')-hydroxyl group of taxane esters)
RN 179798-21-1 CAPLUS
CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



DOCUMENT NUMBER: 142:411508
TITLE: Method for inverting the C(2')-hydroxyl group of taxane esters
INVENTOR(S): Mcchesney, James D.; Chander, Madhavi C.; Henri, John T.; Ferrara, James V.; Brinkman, Herbert R.
PATENT ASSIGNEE(S): Mayne Pharma USA, Inc., USA
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037840	A1	20050428	WO 2004-US33858	20041014

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-511888P P 20031016
OTHER SOURCE(S): CASREACT 142:411508; MARPAT 142:411508
GI

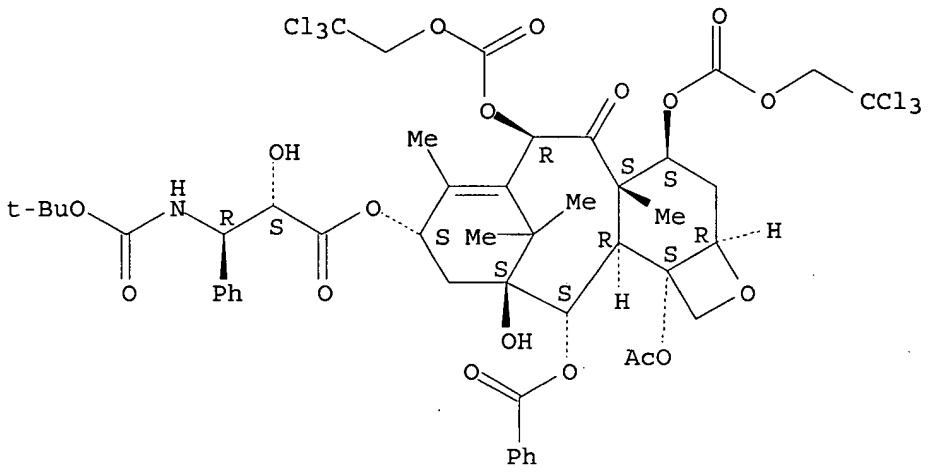
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides a method for inverting the 2'-hydroxy position of selected taxanes via cyclization of the side chain into an oxazole. The method comprises: protecting the 2' hydroxyl group of a first selected taxane I [P = H, R1 = alkyl, olefin, aromatic, O-alkly, O-olefin, O-aromatic; R2 = H, alkyl, olefin, aromatic; R3 = taxane backbone (e.g., Baccatin III)] with a hydroxyl protecting group, such as a sulfonate. The protected taxane compound I [P = tosyl, mesyl, nosyl] is then converted to an oxazole compound II having an oxazole ring. The oxazole ring is then opened by an appropriate process, such as by hydrolyzing the oxazole compound thereby to form an intermediate compound e.g. amine salt III·HA [A = anion of an acid], which is then converted to a second taxane IV. Alternatively, the method may be used to convert the second taxane into the first taxane via intermediates V and VI·HA. The intermediate compound may be an amine salt (III·HA or VI·HA) that is treated with a base to form the second taxane. The method contemplated by be used to convert 2'-epi-paclitaxel into paclitaxel. Alternatively, the method may be used to convert paclitaxel into 2'-epi-paclitaxel. The present invention also relates to novel compds. and intermediates formed by the process.

IT **179551-57-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and benzoyl group migration in; method for inverting the C(2')-hydroxyl group of taxane esters)

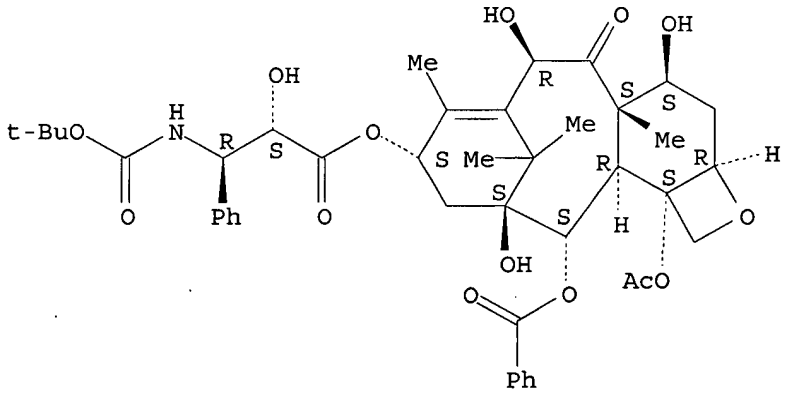
(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4,6-bis[[(2,2,2-trichloroethoxy)carbonyl]oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



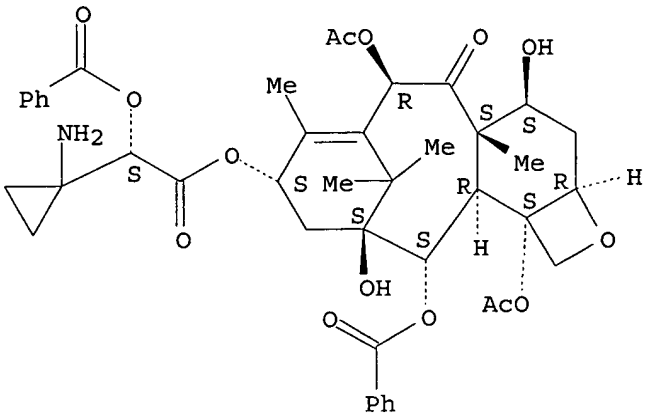
IT **114977-29-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(novel method to synthesize docetaxel and its isomer with high yields)
RN 114977-29-6 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 5 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:371264 CAPLUS



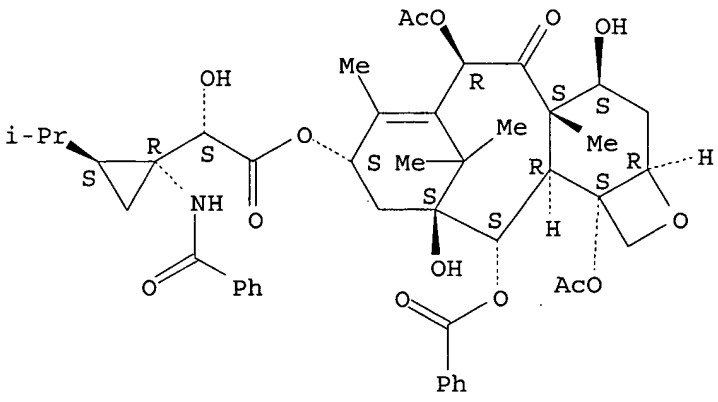
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 4 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:489165 CAPLUS
DOCUMENT NUMBER: 143:153531
TITLE: A novel method to synthesize docetaxel and its isomer with high yields
AUTHOR(S): Qi, Chuan-Min; Wang, Yun-Feng; Yang, Ling-Chun
CORPORATE SOURCE: Department of Chemistry, Beijing Normal University, Beijing, 100875, Peop. Rep. China
SOURCE: Journal of Heterocyclic Chemistry (2005), 42(4), 679-684
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:153531

AB Side chains of docetaxel and its isomer were obtained through Staudinger cycloaddn. and catalytic hydrogenation of chlorophenyl intermediates, using chlorobenzaldehyde as starting material. Syntheses of three novel chiral azetidinone derivs. through the Staudinger cycloaddn. reaction of chlorophenyl chiral amine Schiff base with different substituted positions were described and their ring-opening reaction under the catalysis of Pd/MgCO3 or Pd/C to afford side chains of docetaxel and its isomer in high yields was investigated. Finally, docetaxel and its isomer were obtained. Single crystal of (3S,4R)-3-hydroxy-N-[(S)-(1-phenyl)ethyl]-4-(2'-chlorophenyl)-2-azetidinone was obtained, the configuration of which was determined by X-ray diffraction. Because of the mild cyclization reaction condition and convenient asym. resolution operation when p-chlorobenzaldehyde was employed instead of benzaldehyde, the yield of cyclization and hydrogenation increased dramatically and the total yield of docetaxel was higher than the result in literature. When o-chlorobenzaldehyde was employed instead of benzaldehyde an isomer of docetaxel was obtained by the same way.

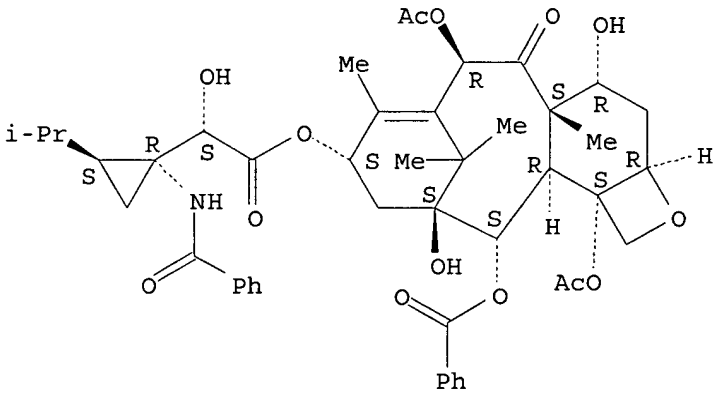
IT **114977-25-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel method to synthesize docetaxel and its isomer with high yields)

RN 114977-25-2 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-



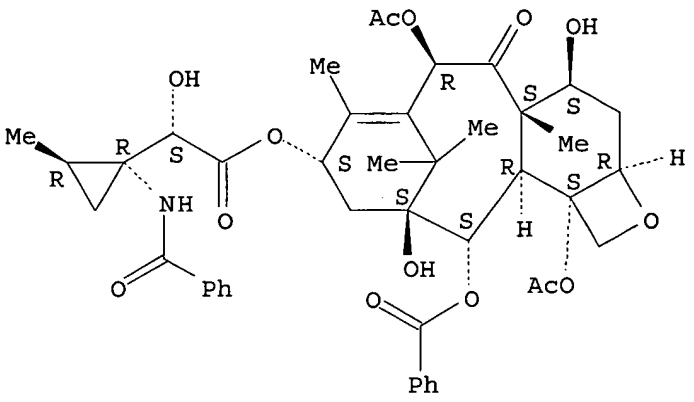
RN 869735-09-1 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-2-(1-methylethyl)-, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



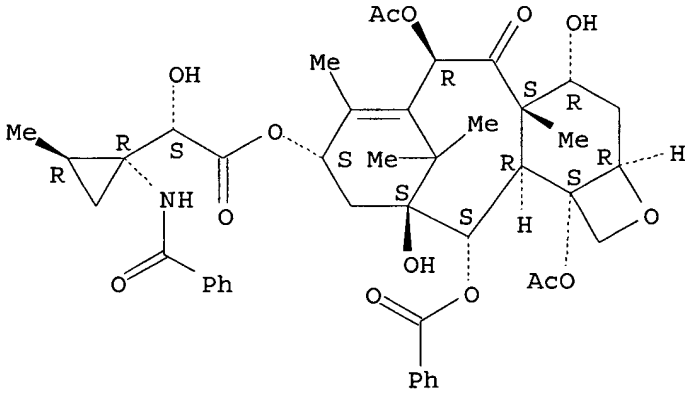
IT **534572-19-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anticancer activity of C3'-cyclopropanated taxol analogs)
RN 534572-19-5 CAPLUS
CN Cyclopropaneacetic acid, 1-amino-α-(benzoyloxy)-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



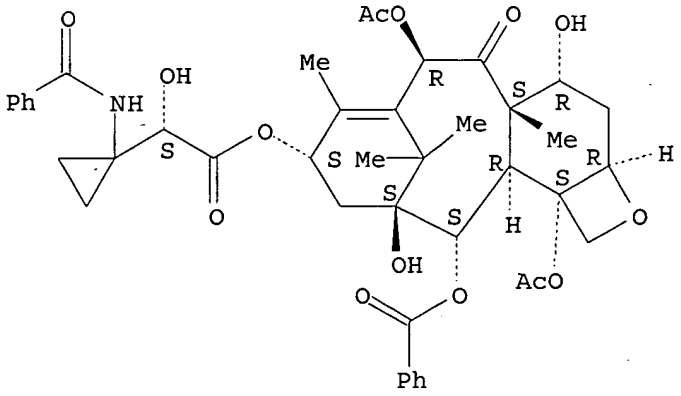
RN 869735-07-9 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-2-methyl-, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 869735-08-0 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-2-(1-methylethyl)-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,1R,2S)- (9CI) (CA INDEX NAME)

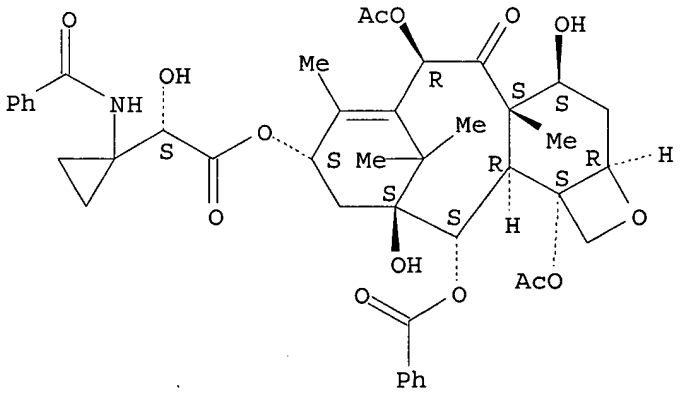
Absolute stereochemistry. Rotation (-).



IT **534572-23-1P 869735-06-8P 869735-07-9P**
869735-08-0P 869735-09-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and anticancer activity of C3'-cyclopropanated taxol analogs)

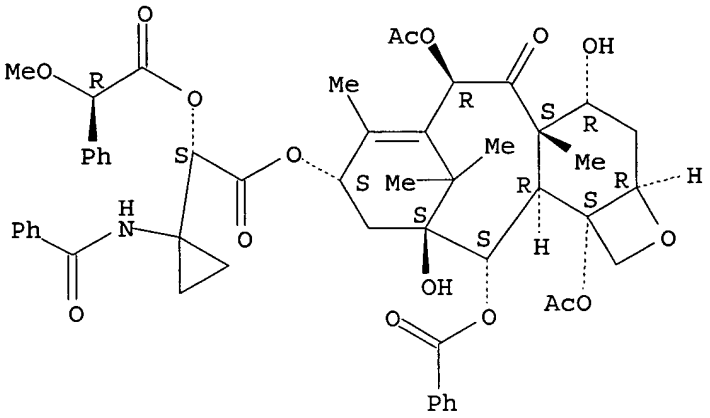
RN 534572-23-1 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



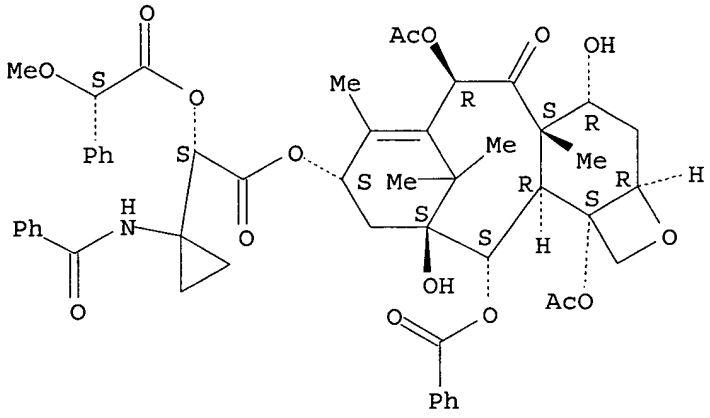
RN 869735-06-8 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-2-methyl-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 534572-30-0 CAPLUS
CN Benzeneacetic acid, α-methoxy-, (1S)-1-[1-(benzoylamino)cyclopropyl]-2-[[(2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl]oxy]-2-oxoethyl ester, (αS)- (9CI) (CA INDEX NAME)

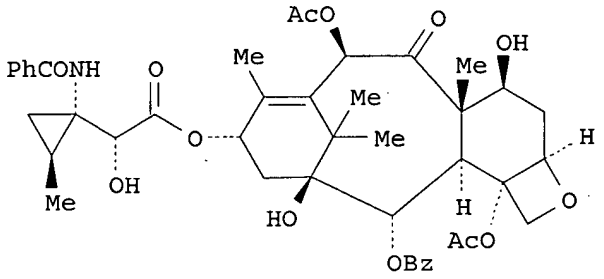
Absolute stereochemistry.



IT **534572-25-3P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anticancer activity of C3'-cyclopropanated taxol analogs)
RN 534572-25-3 CAPLUS
CN Cyclopropaneacetic acid, 1-(benzoylamino)-α-hydroxy-, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Lakdawala, Ami; Snyder, James P.; Bane, Susan L.; Shanker, Natasha; Ravindra, Rudravajhala; Kingston, David G. I.
CORPORATE SOURCE: Department of Chemistry, M/C 0212, Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061, USA
SOURCE: European Journal of Organic Chemistry (2005), (18), 3962-3972
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:6936
GI



I

AB Ten taxoids with a cyclopropanated side chain were synthesized by coupling a spirocyclopropanated oxazoline-5-carboxylic acid with 7-(triethylsilyl)baccatin III, followed by hydrolytic ring opening and benzoyl migration. The absolute configuration of the 2'-position was determined by NMR anal. of the corresponding Mosher esters. These paclitaxel analogs were active in A2780 mammalian and PC-3 prostate cancer cell lines, and also in a tubulin-assembly assay, but all the analogs were less active than paclitaxel itself. To probe the basis for the uniform potency reduction shown by the cyclopropanated taxoid series, we have examined the conformational properties of compound I alone by mol. mechanics and in complex with tubulin by mol. dynamics. In addition, we have performed an NMR/NAMFIS conformer deconvolution anal. for compound I. Both modeling and NAMFIS approaches provide a satisfying understanding of the biol. behavior of the series of cyclopropanated taxoids and provide further, though indirect, support for the T-form as characteristic of taxoids bound to β-tubulin.

IT **534572-29-7P 534572-30-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and absolute configuration of)

RN 534572-29-7 CAPLUS

CN Benzeneacetic acid, α-methoxy-, (1S)-1-[1-(benzoylamino)cyclopropyl]-2-[[(2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl]oxy]-2-oxoethyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

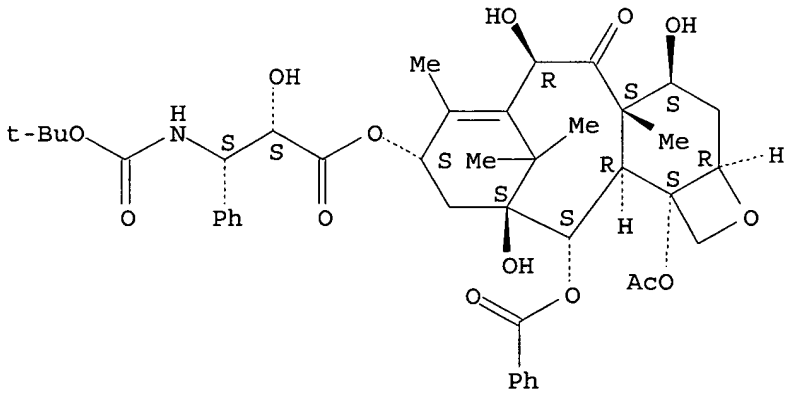
AUTHOR(S): Xu, Xuan; Xu, Zhi-guang; Luo, Yi-fan
CORPORATE SOURCE: School of Chemistry and Environment, South China Normal University, Guangzhou, 510631, Peop. Rep. China
SOURCE: Huanan Shifan Daxue Xuebao, Ziran Kexueban (2005), (4), 73-80
CODEN: HSDZER; ISSN: 1000-5463
PUBLISHER: Huanan Shifan Daxue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB After the MM3 geometry optimizating, the electronic structures of 43 taxol analogs have been calculated by MNDO quantum chemical method. The BP artificial neural network pattern recognition has been performed for analyzing the QSAR of taxol analog anti-tumor drugs. It can be concluded as follows: (1) The relationship between logPT values of C13 side chain in taxol analogs and activity follows the parabola model (Popt = 3.14). The more neg. charge of Bz on 2 - OBz and pos. charge of C1 and C3' atoms of taxol analogs, the higher activities they will have. R1, R2, 1 - OH and 2 - OBz may be the important active sites of the mols. The BP artificial neural network pattern recognition has a 98% accuracy, which may predict the activities of taxol analogs.

IT **133577-33-0**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(neural network pattern recognition study on quant. structure - activity relationships of taxol analog anti-tumor drugs)

RN 133577-33-0 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 3 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1082693 CAPLUS
DOCUMENT NUMBER: 144:6936
TITLE: C-3'-cyclopropanated taxol analogs: Synthesis, bioassay and biostructural analysis
AUTHOR(S): Liu, Changhui; Tamm, Markus; Notzel, Marcus W.; Rauch, Karsten; de Meijere, Armin; Schilling, Jennifer K.;

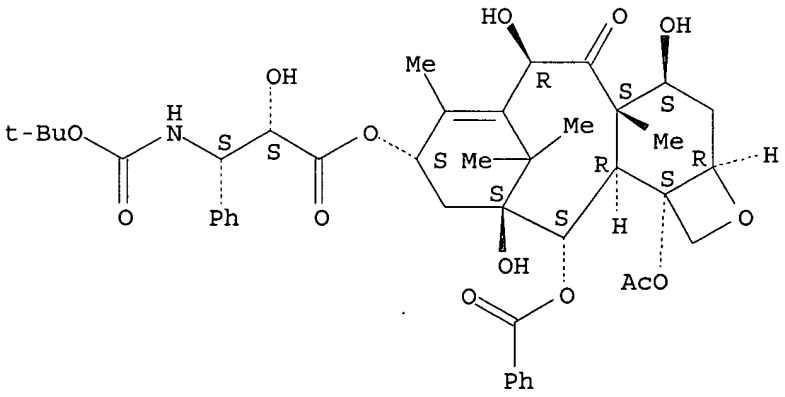
CORPORATE SOURCE: Department of Analytical Research, Discovery Research, Dr. Reddy's Laboratories Ltd., Hyderabad, Andhra Pradesh, 500049, India
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2006), 40(3), 614-622
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB During the process development of docetaxel, two polar impurities (Impurities I and II) and two non-polar impurities (Impurities III and IV) were detected by high performance liquid chromatog. (HPLC). All the impurities were isolated by Medium Pressure Liquid Chromatog. (MPLC). The Impurities I, II, III and IV were identified as 13-[(4S,5R)-2-oxo-4-phenyl-oxazolidine-5-carboxy]-10-deacetyl baccatin III ester, 2'-epi docetaxel, 7-epi docetaxel and 13-[(4S,5R)-2-oxo-4-phenyl-oxazolidine-3,5-dicarboxyl-3-tert-butyl]-10-deacetyl baccatin III ester, resp., based on one- (1D) and two-dimensional (2D) NMR spectroscopy data. The Impurity IV was crystallized and the structure was solved by single crystal X-ray diffraction (XRD). Two impurities (Impurities II and III) were found to be process related, while the remaining two impurities (Impurities I and IV) turned out to be isomers. The formation of these impurities was discussed.

IT **133577-33-0**
RL: ANT (Analyte); ANST (Analytical study)
(determination of impurities in docetaxel by HPLC)

RN 133577-33-0 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 52 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:46697 CAPLUS
DOCUMENT NUMBER: 144:460276
TITLE: Neural network pattern recognition study on the quantitative structure - activity relationships of taxol analogue anti-tumor drugs

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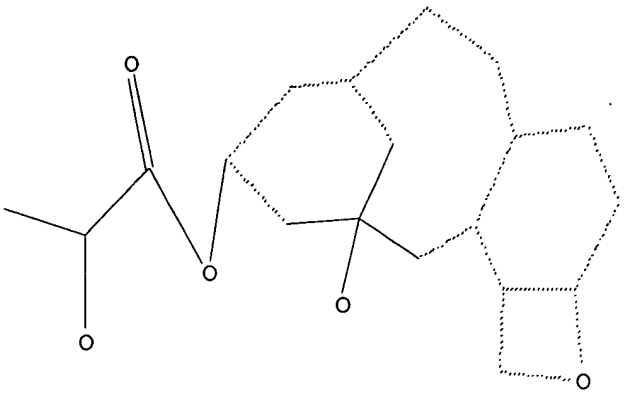

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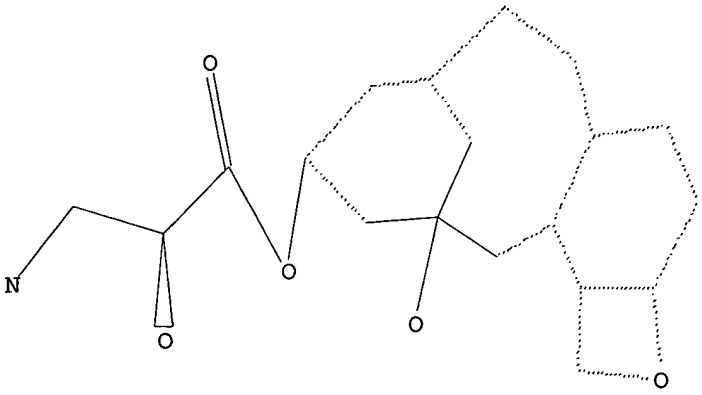

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Structure attributes must be viewed using STN Express query preparation.
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L24           59 SEA FILE=CAPLUS ABB=ON  PLU=ON  L22


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L51          52 L24 NOT L49

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L51  ANSWER 1 OF 52  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2006:160274  CAPLUS
DOCUMENT NUMBER:          144:419879
TITLE:                    Isolation and characterization of impurities in
                          docetaxel
AUTHOR(S):                Vasu Dev, R.; Moses Babu, J.; Vyas, K.; Sai Ram, P.;
                          Ramachandra, P.; Sekhar, N. M.; Mohan Reddy, D. N.;
                          Srinivasa Rao, N.
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FILE COVERS 1907 - 19 Sep 2006 VOL 145 ISS 13
FILE LAST UPDATED: 18 Sep 2006 (20060918/ED)

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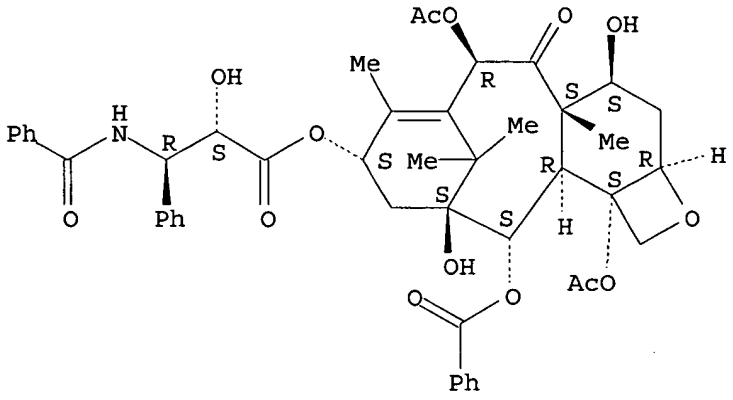

IC ICM C07D305-14
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 63
IT 114977-28-5P, Taxotere **149197-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

CS	1994-661	A 19920922
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EP	1998-114788	A3 19920922
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WO	1992-US7952	A 19920922
US	1992-967998	B1 19921026
WO	1994-US2382	W 19940304
US	1994-263270	B1 19940621
US	1994-314532	A1 19940928
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US	1995-483309	A3 19950607
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OTHER SOURCE(S): MARPAT 119:117582.

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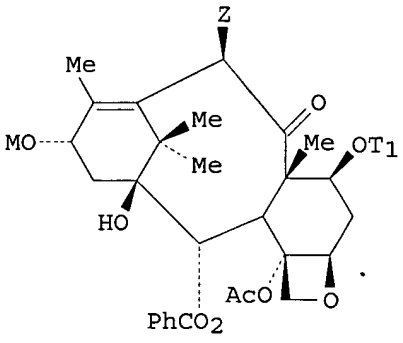

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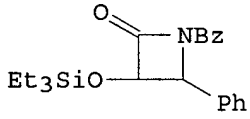

II

AB A metal alkoxide I (T1 = H, hydroxy protecting group; Z = OT2, O2CMe; T2 = H, hydroxy protecting group; M = Group IA, IIA, transition metal) are useful in the preparation of biol. active derivs. of baccatin III and 10-deacetylbaccatin III. Thus, treating 7-(triethylsilyl)baccatin III with K hexamethyldisilazide followed by azetidinone II gave 90% (2'R,3'S)-2',7-bis(triethylsilyl)taxol.

IT **149197-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 149197-23-9 CAPLUS

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CA 2254273	AA	19920922	CA 1992-2254273	19920922
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US 7074945	B2	20060711		
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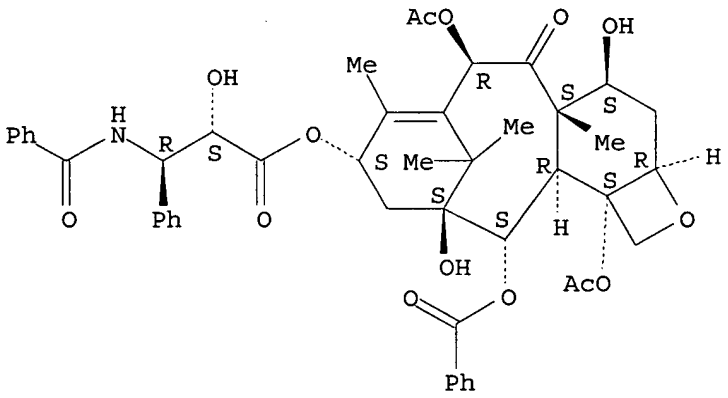
			US 1992-863849	A 19920406
			US 1992-900408	A 19920618
			CA 1992-2077394	A3 19920902
			CA 1992-2098478	A3 19920922
			CS 1994-660	A 19920922

CN Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αS,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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ICS C07C229-10; C07C229-34; C07D305-14; C07D307-42; C07D307-46; C07D307-52; C07D317-50; C07D407-12; C07D409-12
CC 30-20 (Terpenes and Terpenoids)
IT 33069-62-4P, Taxol **149197-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from (triethylsilyl)baccatin III and azetidinone derivative)

L49 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:517582 CAPLUS
DOCUMENT NUMBER: 119:117582
TITLE: Metal alkoxides of baccatin III
INVENTOR(S): **Holton, Robert A.**
PATENT ASSIGNEE(S): Florida State University, USA
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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ZA 9206829	A	19930315	ZA 1992-6829	19920908
ZA 9207038	A	19930514	ZA 1992-7038	19920915
ZA 9207039	A	19931220	ZA 1992-7039	19920915
IL 103192	A1	19970610	IL 1992-103192	19920916

US 6683196	B2	20040127			
JP 2004043439	A2	20040212	JP 2003-128200		20030506
US 2004073048	A1	20040415	US 2003-673897		20030929
US 7074945	B2	20060711			
PRIORITY APPLN. INFO.:			US 1991-763805	A	19910923
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OTHER SOURCE(S): MARPAT 119:139574

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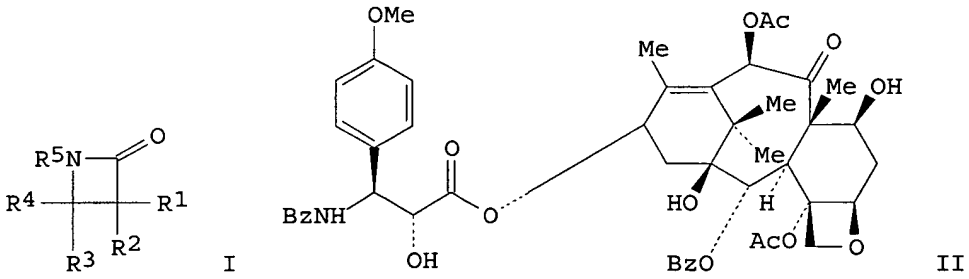

AB A metal alkoxide MOCE1E2E3 (M = alkali metal, E1, E2, E3 = H, aliphatic, aryl, alkanoyloxy) is reacted with a β-lactam I [R1 = (un)protected OH, SH, NH2, R2 = H, aliphatic, aryl, heteroaryl, R3, R4 = aliphatic, aryl, heteroaryl, acyl, R5 = acyl, carboxy, thiocarboxy, amido, sulfonyl, phosphoryl] to give isoserine esters R5NHCR3R4CR1R2CO2CE1E2E3 which are reacted with a metal derivative of a taxol derivative to give appropriately substituted isoserine esters, e.g. II.

IT **149197-23-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from (triethylsilyl)baccatin III and azetidinone derivative)

RN 149197-23-9 CAPLUS

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

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CA 2221190	C	20020212		
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ZA 9207038	A	19930514	ZA 1992-7038	19920915
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CA 2254273	C	20030325		
CA 2098478	AA	19930324	CA 1992-2098478	19920922
CA 2098478	C	19990914		
AU 9226890	A1	19930427	AU 1992-26890	19920922
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JP 07502983	T2	19950330	JP 1993-506299	19920922
JP 3469237	B2	20031125		
HU 71795	A2	19960228	HU 1994-830	19920922
EP 884314	A2	19981216	EP 1998-114788	19920922
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EP 884314	B1	20040121		
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CZ 287609	B6	20010117	CZ 1994-661	19920922
EP 1193252	A2	20020403	EP 2002-688	19920922
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US 6479678	B1	20021112	US 2000-517791	20000302
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US 2003027855	A1	20030206	US 2002-208418	20020730
US 6710191	B2	20040323		
US 2003120096	A1	20030626	US 2002-289103	20021106

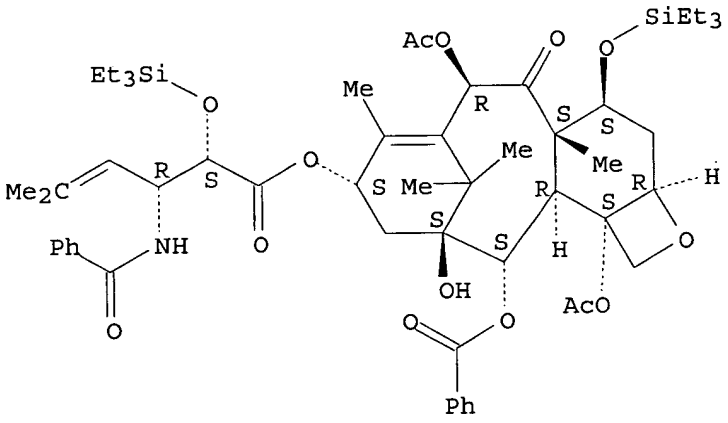
AB Taxane derivs. I [R1 is butenyl, R3 is Ph, T1 is hydrogen, hydroxyl protecting group, or COT2, T2 is H, C1-C6 alkyl, C2-C6 alkenyl, C2-C6 alkynyl or monocyclic aryl, Ac is acetyl, and E1 and E2 are independently selected from hydrogen and hydroxyl protecting groups] are prepared as antitumor agents. Treatment of 7-triethylsilyl baccatin III with BuLi, followed by reaction with cis-1-benzoyl-3-triethylsilyloxy-4-(2-methyl-1-propenyl)azetidin-2-one and hydrolysis in the presence of HF and pyridine, gave 3'-desphenyl-3'-(2-methyl-1-propenyl) taxol (II). II in vitro showed IC50 of 0.001 (unit unspecified) against human colon carcinoma cells HCT-116, vs. 0.004 for taxol.

IT **155897-88-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 155897-88-4 CAPLUS

CN 4-Hexenoic acid, 3-benzoyl-5-methyl-2-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9a(2S*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-335
ICS C07D305-14

INCL 514449000

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT **155897-88-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L49 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:539574 CAPLUS

DOCUMENT NUMBER: 119:139574

TITLE: Preparation of substituted isoserine esters using metal alkoxides and (beta)-lactams

INVENTOR(S): **Holton, Robert A.**

PATENT ASSIGNEE(S): Florida State University, USA

SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2

US 2004073048	A1	20040415	US 2003-673897		20030929
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OTHER SOURCE(S): MARPAT 121:35197

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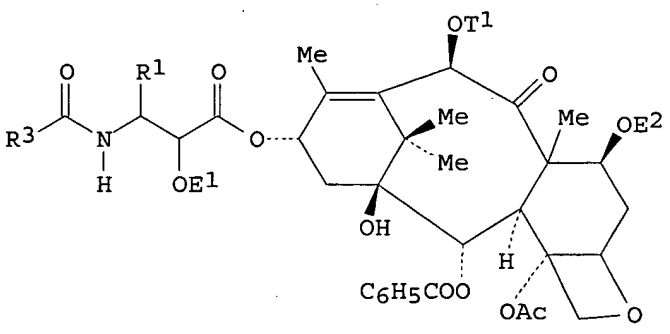

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IL 103191	A1	20010724	IL 1992-103191	19920916
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EP 884314	A3	20020502		
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EP 1193252	A2	20020403	EP 2002-688	19920922
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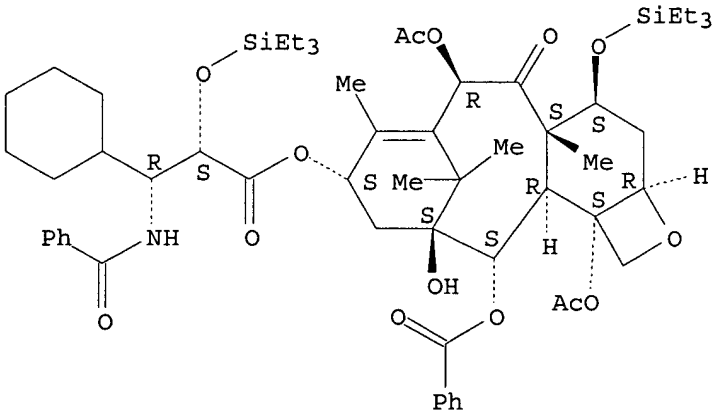
TW 420670	B	20010201	TW 1994-83103428	19940418
US 5574156	A	19961112	US 1994-254561	19940606
US 5466834	A	19951114	US 1994-314532	19940928
US 5539103	A	19960723	US 1994-351532	19941207
US 5728850	A	19980317	US 1995-463704	19950605
US 5723634	A	19980303	US 1995-483309	19950607
US 6066747	A	20000523	US 1995-522307	19951030
AU 9726210	A1	19970918	AU 1997-26210	19970623
AU 706985	B2	19990701		
US 6069260	A	20000530	US 1997-941640	19970930
US 6005138	A	19991221	US 1997-989990	19971212
CN 1270958	A	20001025	CN 1999-118060	19990818
US 6395895	B1	20020528	US 1999-427973	19991027
US 6479678	B1	20021112	US 2000-517791	20000302
US 2001014746	A1	20010816	US 2001-804821	20010313
US 6562962	B2	20030513		
US 2003027855	A1	20030206	US 2002-208418	20020730
US 6710191	B2	20040323		
US 2003120096	A1	20030626	US 2002-289103	20021106
US 6683196	B2	20040127		
JP 2004043439	A2	20040212	JP 2003-128200	20030506

CN Cyclohexanepropanoic acid, β-(benzoylamino)-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-335
ICS C07D305-14
INCL 514449000
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1
IT **156767-25-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

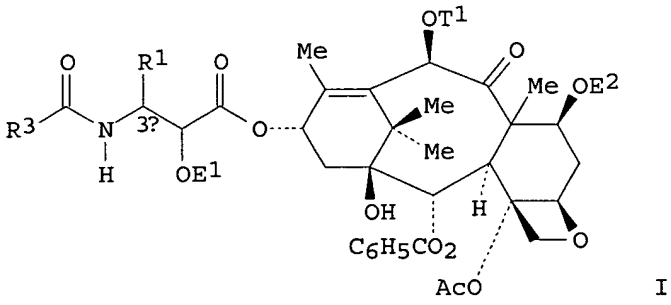
L49 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:435197 CAPLUS
DOCUMENT NUMBER: 121:35197
TITLE: Preparation of butenyl substituted taxanes as antitumor agents
INVENTOR(S): **Holton, Robert A.**; Nadizadeh, Hossain
PATENT ASSIGNEE(S): Florida State University, USA
SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 949,107.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5284864	A	19940208	US 1992-975705	19921113
CA 2221190	AA	19920902	CA 1992-2221190	19920902
CA 2221190	C	20020212		
ZA 9206827	A	19930315	ZA 1992-6827	19920908
ZA 9206828	A	19930315	ZA 1992-6828	19920908
ZA 9206829	A	19930315	ZA 1992-6829	19920908
ZA 9207038	A	19930514	ZA 1992-7038	19920915
ZA 9207039	A	19931220	ZA 1992-7039	19920915

CS	1994-660	A 19920922
CS	1994-661	A 19920922
EP	1992-921316	A3 19920922
EP	1998-114788	A3 19920922
JP	1993-506299	A3 19920922
US	1992-967998	B1 19921026
US	1992-968003	A3 19921026
US	1992-976331	A 19921113
US	1993-5229	A 19930115
US	1993-10798	A 19930129
US	1993-26978	A 19930305
US	1993-34247	A 19930322
US	1993-94756	A 19930720
EP	1994-901360	A3 19931101
WO	1993-US10816	W 19931101
WO	1994-US2382	W 19940304
US	1994-263270	B1 19940621
US	1994-314532	A1 19940928
US	1994-351532	A3 19941207
US	1995-462125	A1 19950605
US	1995-483309	A3 19950607
US	1996-607108	A1 19960226
US	1997-941640	A1 19970930
US	2000-517791	A1 20000302
US	2000-566970	A1 20000509
US	2002-134762	A3 20020429
US	2002-194343	A1 20020712
US	2002-289103	A1 20021106

OTHER SOURCE(S): MARPAT 121:109330

GI



I

AB Taxane derivs. (I; R1 = cyclohexyl; R3 = Ph; T1 = H, hydroxyl protecting group, or -COT2, T2 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl or monocyclic aryl; E1, E2 = H, functional groups which increase water solubility), were prepared Thus, 7-triethylsilylbaccatin III in THF at -45° was treated with BuLi and then cis-1-benzoyl-3-triethylsilyloxy-4-cyclohexylazetidine-2-one; the mixture was warmed to 0° and stirred 1h to give (2'R,3'S)-2',7-bistriethylsilyl-3'-desphenyl-3'-cyclohexyltaxol, which was stirred with aqueous HF and pyridine in acetonitrile to give 73% 3'-desphenyl-3'-cyclohexyltaxol (II). II and taxol showed IC50 = 0.100 and 0.536, resp., against HCT116/VM46.

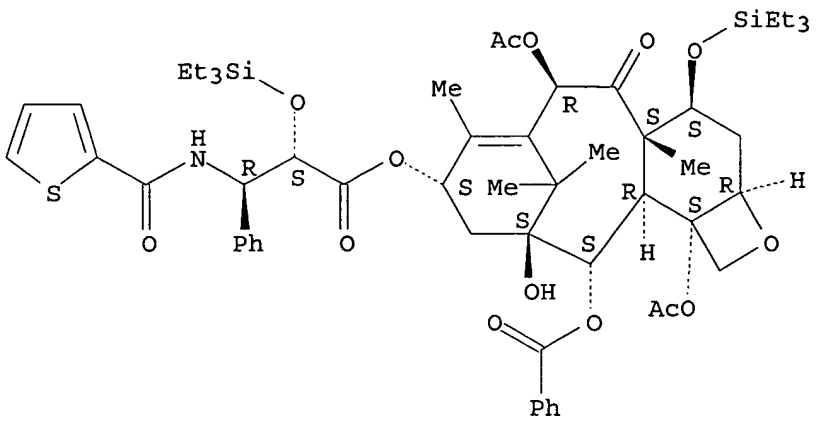
IT **156767-25-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 156767-25-8 CAPLUS

CZ 287609	B6	20010117	CZ 1994-661	19920922	
EP 1193252	A2	20020403	EP 2002-688	19920922	
EP 1193252	A3	20031105			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE					
SG 97130	A1	20030718	SG 1999-4181	19920922	
CN 1075315	A	19930818	CN 1992-112286	19920923	
CN 1048982	B	20000202			
CA 2147854	AA	19940526	CA 1993-2147854	19931101	
CA 2147854	C	20060321			
WO 9410997	A1	19940526	WO 1993-US10816	19931101	
W: AU, CA, FI, HU, JP, KR, NO, NZ, PL, RU					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
AU 9455976	A1	19940608	AU 1994-55976	19931101	
AU 689451	B2	19980402			
EP 667772	A1	19950823	EP 1994-901360	19931101	
EP 667772	B1	20030514			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
JP 08503219	T2	19960409	JP 1994-512299	19931101	
EP 1146043	A1	20011017	EP 2001-117886	19931101	
EP 1146043	B1	20060308			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE					
AT 240099	E	20030515	AT 1994-901360	19931101	
PT 667772	T	20030930	PT 1994-901360	19931101	
ES 2199955	T3	20040301	ES 1994-901360	19931101	
AT 319698	E	20060315	AT 2001-117886	19931101	
ZA 9308216	A	19940722	ZA 1993-8216	19931103	
CN 1092417	A	19940921	CN 1993-112765	19931113	
CN 1075066	B	20011121			
TW 396159	B	20000701	TW 1994-83103422	19940418	
TW 411331	B	20001111	TW 1994-83103456	19940419	
US 5574156	A	19961112	US 1994-254561	19940606	
US 5466834	A	19951114	US 1994-314532	19940928	
US 5539103	A	19960723	US 1994-351532	19941207	
US 6335362	B1	20020101	US 1995-462125	19950605	
US 5723634	A	19980303	US 1995-483309	19950607	
US 6066747	A	20000523	US 1995-522307	19951030	
US 6069260	A	20000530	US 1997-941640	19970930	
CN 1285351	A	20010228	CN 1999-124858	19991115	
US 6479678	B1	20021112	US 2000-517791	20000302	
US 2001014746	A1	20010816	US 2001-804821	20010313	
US 6562962	B2	20030513			
US 2003027855	A1	20030206	US 2002-208418	20020730	
US 6710191	B2	20040323			
US 2003120096	A1	20030626	US 2002-289103	20021106	
US 6683196	B2	20040127			
US 2003187061	A1	20031002	US 2003-351837	20030127	
JP 2004043439	A2	20040212	JP 2003-128200	20030506	
US 2004073048	A1	20040415	US 2003-673897	20030929	
US 7074945	B2	20060711			

PRIORITY APPLN. INFO.:

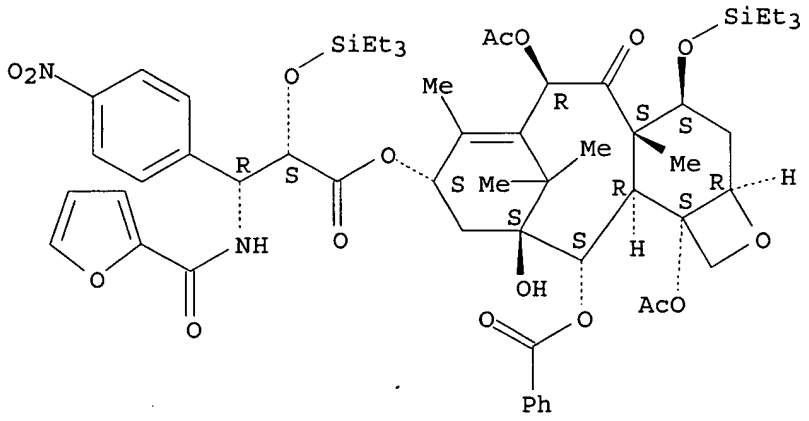
US 1991-763805	B2	19910923
US 1992-862955	B2	19920403
US 1992-863849	B2	19920406
US 1992-949107	A2	19920922
US 1989-359634	YY	19890531
US 1989-415028	A1	19890929
US 1992-863451	A	19920403
US 1992-863840	A	19920406
US 1992-900408	A	19920618
CA 1992-2077394	A3	19920902
CA 1992-2098478	A3	19920922



IC ICM A61K031-34
ICS A61K031-38; C07D305-14
INCL 514444000
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1
IT 157187-81-0P 157187-82-1P 157187-83-2P **157241-41-3P**
157241-42-4P 157241-43-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in preparation of neoplasm inhibitor)

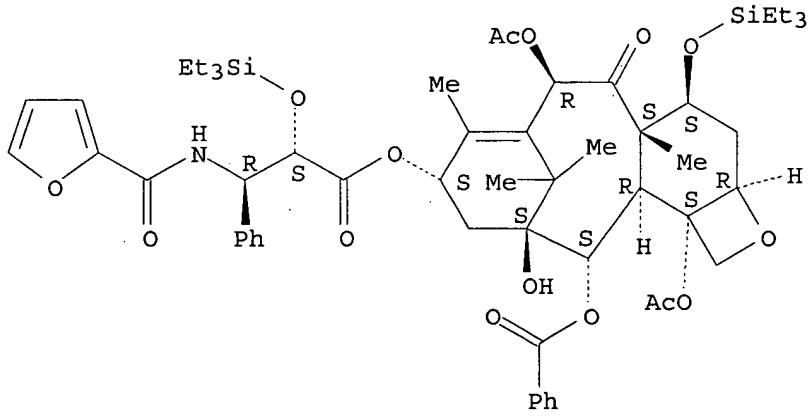
L49 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:509330 CAPLUS
DOCUMENT NUMBER: 121:109330
TITLE: Preparation of cyclohexyl-substituted taxanes as anticancer drugs.
INVENTOR(S): **Holton, Robert A.**; Nadizadeh, Hossain
PATENT ASSIGNEE(S): Florida State University, USA
SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 949,107.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5284865	A	19940208	US 1992-976331	19921113
CA 2221190	AA	19920902	CA 1992-2221190	19920902
CA 2221190	C	20020212		
ZA 9206827	A	19930315	ZA 1992-6827	19920908
ZA 9206828	A	19930315	ZA 1992-6828	19920908
ZA 9206829	A	19930315	ZA 1992-6829	19920908
ZA 9207038	A	19930514	ZA 1992-7038	19920915
ZA 9207039	A	19931220	ZA 1992-7039	19920915
IL 103191	A1	20010724	IL 1992-103191	19920916
CA 2254273	AA	19920922	CA 1992-2254273	19920922
CA 2254273	C	20030325		
EP 884314	A2	19981216	EP 1998-114788	19920922
EP 884314	A3	20020502		
EP 884314	B1	20040121		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE				
CZ 287417	B6	20001115	CZ 1994-660	19920922



RN 157241-42-4 CAPLUS
CN Benzenepropanoic acid, β-[(2-furanylcarbonyl)amino]-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157241-43-5 CAPLUS
CN Benzenepropanoic acid, β-[(2-thienylcarbonyl)amino]-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

JP 1993-506299	A3	19920922
US 1992-967998	B1	19921026
US 1992-968003	A3	19921026
US 1992-975723	A	19921113
US 1993-34247	A2	19930322
US 1993-34852	B2	19930322
US 1993-94566	B1	19930720
WO 1993-US10473	W	19931101
WO 1994-US2382	W	19940304
US 1994-263270	B1	19940621
US 1994-314532	A1	19940928
US 1994-351532	A3	19941207
US 1995-462122	A3	19950605
US 1995-483309	A3	19950607
US 1996-607108	A1	19960226
US 1997-941640	A1	19970930
US 1997-953889	A1	19971020
US 2000-517791	A1	20000302
US 2000-566970	A1	20000509
US 2002-194343	A1	20020712
US 2002-289103	A1	20021106

OTHER SOURCE(S): MARPAT 121:134497
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. (I; R1 = Ph, p-nitrophenyl; R3 = furyl, thienyl; T1 = H, hydroxyl protecting group, COT2; T2 = H, alkyl, alkenyl, alkynyl, monocyclic aryl; E1, E2 = H, functional groups which increase the water solubility of the taxane derivative), were prepared as antitumor agents. Thus, 7-triethylsilylbaccatin III in THF at -45° was treated with BuLi and then with cis-1-furoyl-3-triethylsilyloxy-4-(4-nitrophenyl)azetidin-2-one followed by stirring to 0° to give a coupling product as a mixture of diastereomers. The crude product was treated with HF in acetonitrile/pyridine to give title compound II. II inhibited HCT 116 and HCT VM46 human colon carcinoma cells with IC50 = 0.002 and 0.883, resp. (no units given).

IT **157241-41-3P 157241-42-4P 157241-43-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in preparation of neoplasm inhibitor)

RN 157241-41-3 CAPLUS

CN Benzenepropanoic acid, β-[(2-furanylcarbonyl)amino]-4-nitro-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE					
CZ 287417	B6	20001115	CZ 1994-660		19920922
CZ 287609	B6	20010117	CZ 1994-661		19920922
EP 1193252	A2	20020403	EP 2002-688		19920922
EP 1193252	A3	20031105			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE					
SG 97130	A1	20030718	SG 1999-4181		19920922
CN 1075315	A	19930818	CN 1992-112286		19920923
CN 1048982	B	20000202			
CA 2147859	AA	19940526	CA 1993-2147859		19931101
WO 9411362	A1	19940526	WO 1993-US10473		19931101
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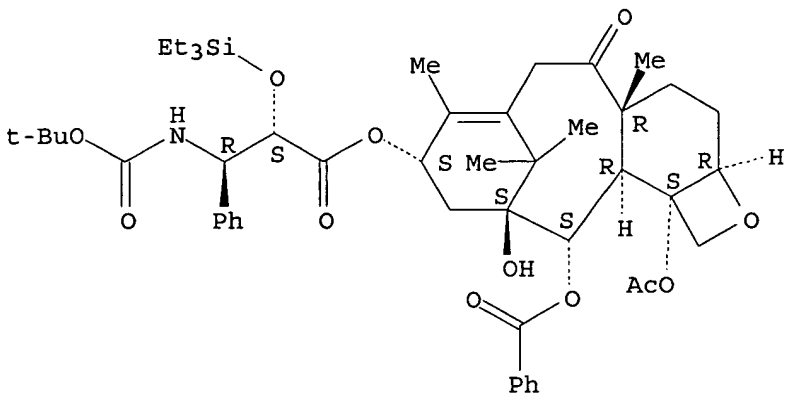
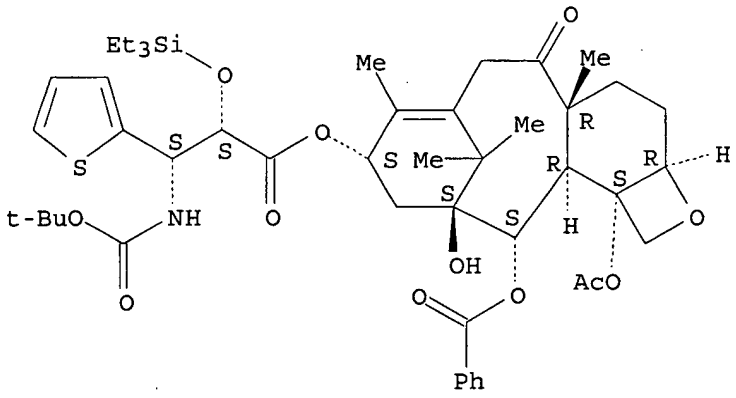
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
AU 9455450	A1	19940608	AU 1994-55450		19931101
AU 682161	B2	19970925			
EP 669918	A1	19950906	EP 1994-900474		19931101
EP 669918	B1	19990203			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
JP 08502995	T2	19960402	JP 1994-512149		19931101
JP 3328286	B2	20020924			
AT 176466	E	19990215	AT 1994-900474		19931101
ES 2130390	T3	19990701	ES 1994-900474		19931101
ZA 9308214	A	19940719	ZA 1993-8214		19931103
IL 107553	A1	19971120	IL 1993-107553		19931110
CN 1094401	A	19941102	CN 1993-114654		19931113
CN 1051310	B	20000412			
TW 396159	B	20000701	TW 1994-83103422		19940418
US 5574156	A	19961112	US 1994-254561		19940606
US 5466834	A	19951114	US 1994-314532		19940928
US 5539103	A	19960723	US 1994-351532		19941207
US 5723634	A	19980303	US 1995-483309		19950607
US 6066747	A	20000523	US 1995-522307		19951030
US 6069260	A	20000530	US 1997-941640		19970930
US 6479678	B1	20021112	US 2000-517791		20000302
US 6369244	B1	20020409	US 2000-523535		20000310
US 2001014746	A1	20010816	US 2001-804821		20010313
US 6562962	B2	20030513			
US 2003027855	A1	20030206	US 2002-208418		20020730
US 6710191	B2	20040323			
US 2003120096	A1	20030626	US 2002-289103		20021106
US 6683196	B2	20040127			
JP 2004043439	A2	20040212	JP 2003-128200		20030506
US 2004073048	A1	20040415	US 2003-673897		20030929
US 7074945	B2	20060711			
PRIORITY APPLN. INFO.:			US 1991-763805	B2	19910923
			US 1992-862955	B2	19920403
			US 1992-863849	B2	19920406
			US 1992-949107	A2	19920922
			US 1989-359634	YY	19890531
			US 1989-415028	A1	19890929
			US 1992-862819	A2	19920403
			US 1992-863451	A	19920403
			US 1992-863840	A	19920406
			US 1992-900408	A	19920618
			CA 1992-2077394	A3	19920902
			CA 1992-2098478	A3	19920922
			CS 1994-660	A	19920922
			CS 1994-661	A	19920922
			EP 1992-921316	A3	19920922
			EP 1998-114788	A3	19920922



IC ICM A61K031-355
ICS C07D305-14
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1
IT **159406-32-3P 159406-33-4P 159406-34-5P**
159406-35-6P 159406-36-7P 159406-37-8P
159406-38-9P 159406-39-0P 159406-40-3P
159406-41-4P 159406-42-5P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; preparation of C-10 taxane derivs. as antileukemia and antitumor agents)

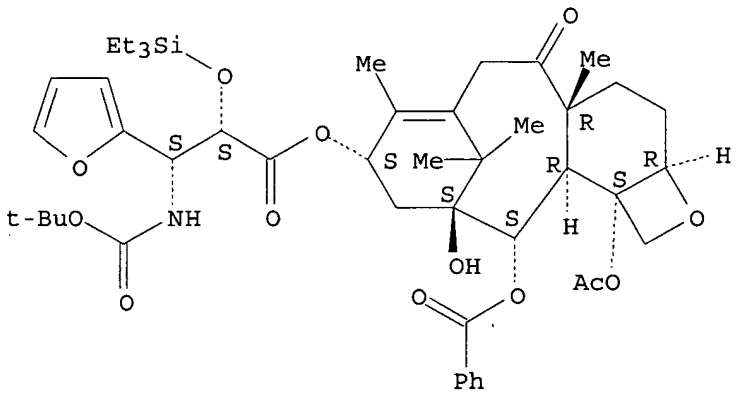
L49 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:534497 CAPLUS
DOCUMENT NUMBER: 121:134497
TITLE: Preparation of furylcarbonyl- or thienylcarbonyl-substituted taxanes as neoplasm inhibitors.
INVENTOR(S): **Holton, Robert A.**; Rengan, Kasthuri; Nadizadeh, Hossain
PATENT ASSIGNEE(S): Florida State University, USA
SOURCE: U.S., 13 pp. Cont.-in-part of U.S. Ser. No. 949,107.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5283253	A	19940201	US 1992-975723	19921113
CA 2221190	AA	19920902	CA 1992-2221190	19920902
CA 2221190	C	20020212		
ZA 9206827	A	19930315	ZA 1992-6827	19920908
ZA 9206828	A	19930315	ZA 1992-6828	19920908
ZA 9206829	A	19930315	ZA 1992-6829	19920908
ZA 9207038	A	19930514	ZA 1992-7038	19920915
ZA 9207039	A	19931220	ZA 1992-7039	19920915
IL 103191	A1	20010724	IL 1992-103191	19920916
CA 2254273	AA	19920922	CA 1992-2254273	19920922
CA 2254273	C	20030325		
EP 884314	A2	19981216	EP 1998-114788	19920922
EP 884314	A3	20020502		
EP 884314	B1	20040121		



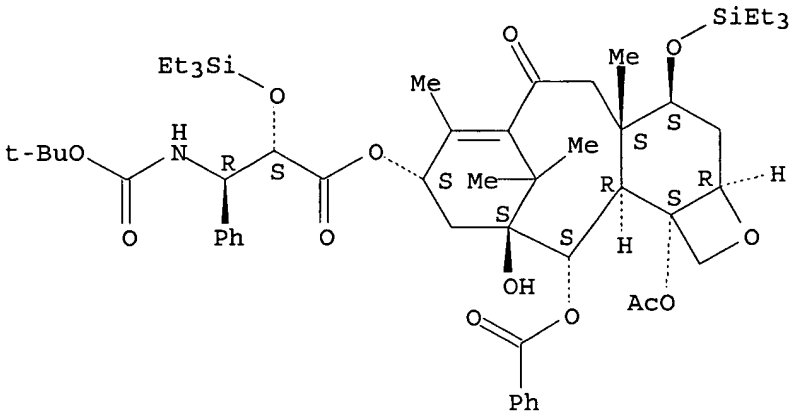
RN 159406-41-4 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4aβ,9α(αS*,βS*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



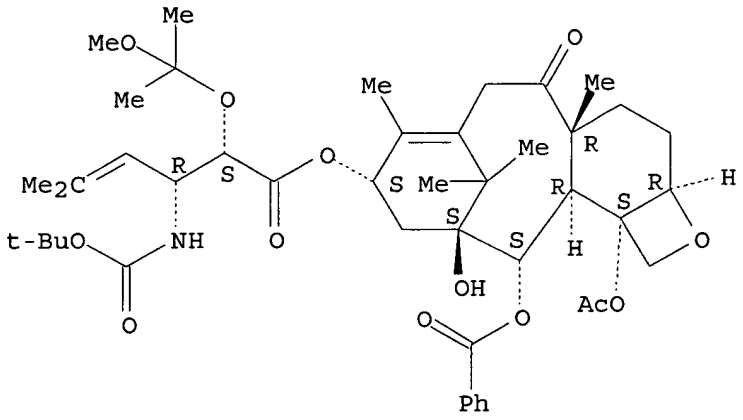
RN 159406-42-5 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4aβ,9α(αS*,βR*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159406-39-0 CAPLUS
CN 4-Hexenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methoxy-1-methylethoxy)-5-methyl-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4aβ,9α(2S*,3R*),11α,12α,12a.alpha.,12bα]]- (9CI) (CA INDEX NAME)

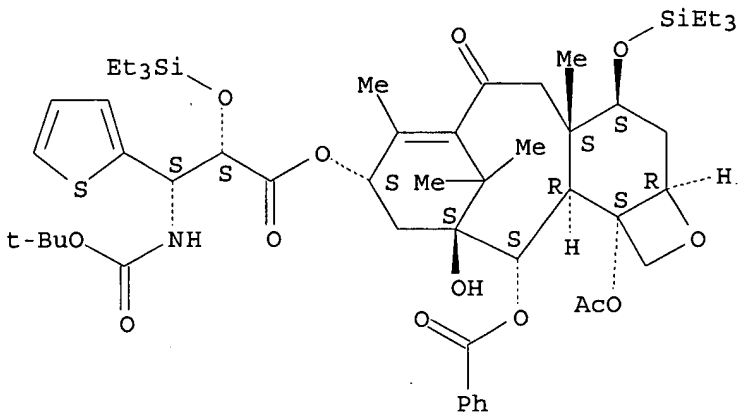
Absolute stereochemistry.



RN 159406-40-3 CAPLUS
CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4aβ,9α(αS*,βS*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

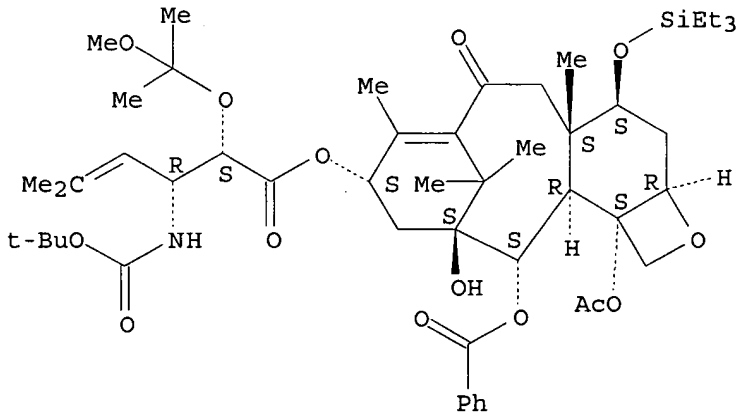
Absolute stereochemistry.

Absolute stereochemistry.



RN 159406-37-8 CAPLUS
CN 4-Hexenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methoxy-1-methylethoxy)-5-methyl-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-6-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(2S*,3R*),11α,12α,12a.alpha.,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

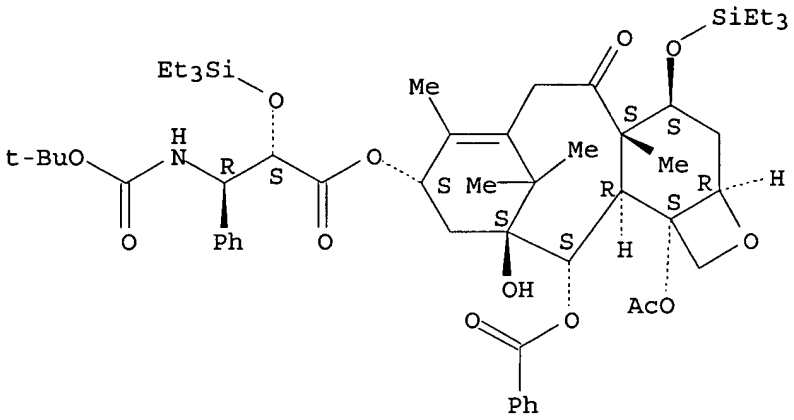


RN 159406-38-9 CAPLUS
CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-6-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βR*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

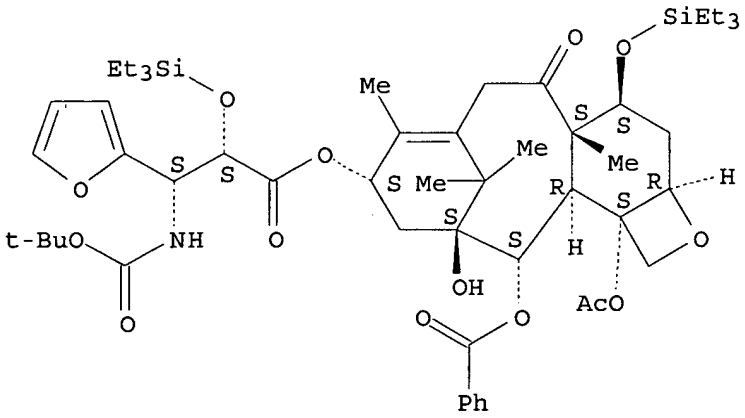
cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βR*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159406-35-6 CAPLUS
CN 2-Furanpropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βS*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

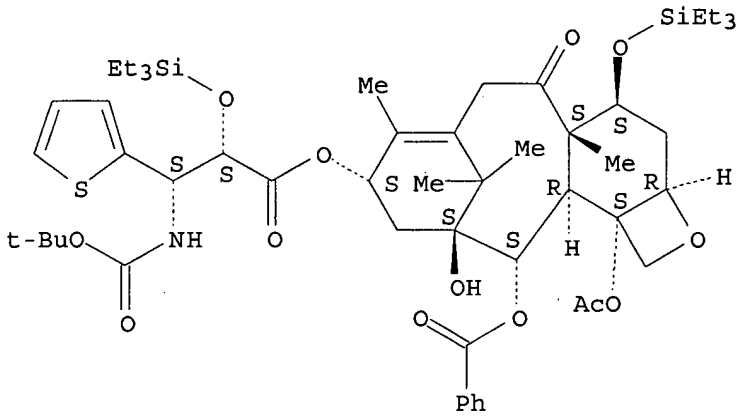
Absolute stereochemistry.



RN 159406-36-7 CAPLUS
CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-6-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βS*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

CN 2-Thiophenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(αS*,βS*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

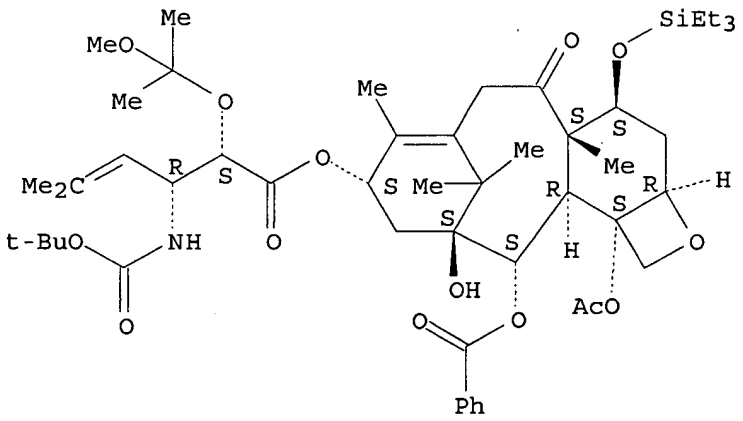
Absolute stereochemistry.



RN 159406-33-4 CAPLUS

CN 4-Hexenoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methoxy-1-methylethoxy)-5-methyl-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,9α(2S*,3R*),11α,12α,12a.alpha.,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



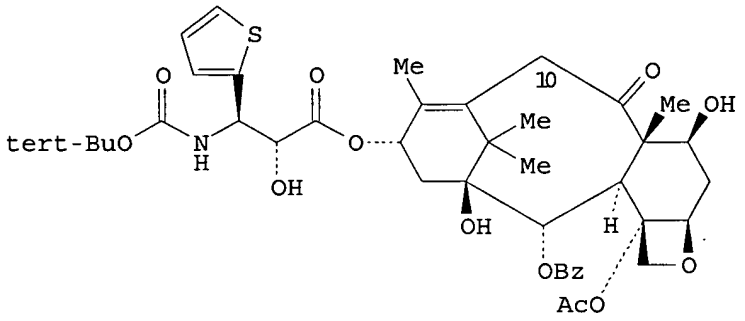
RN 159406-34-5 CAPLUS

CN Benzenepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-

US 1993-34852	A	19930322
US 1993-94545	A	19930720
US 1993-10798	A	19930129
US 1993-26978	A	19930305
US 1993-94717	A	19930720
US 1993-95087	A	19930720
US 1993-95160	A	19930720
EP 1994-909453	A3	19940114
WO 1994-US479	W	19940114
EP 1994-909514	A3	19940128
JP 1994-517370	A3	19940128
EP 1994-909840	A3	19940301
WO 1994-US2210	W	19940301
WO 1994-US2382	W	19940304
EP 1994-911675	A3	19940321
EP 1994-910982	A3	19940929
US 2000-566970	A1	20000509

OTHER SOURCE(S): CASREACT 122:187818; MARPAT 122:187818

GI



I

AB Taxane derivs. substituted on the C-10 position with novel substituents (specifically H2 or oxo) are disclosed. A highly complex Markush structure is claimed, and 11 example prepns. are given. The compds. have utility as antileukemia and antitumor agents. For example, lithiation of 7-O-triethylsilyl-10-desacetoxybaccatin (III) with LiN(SiMe3)2 in THF, followed by esterification with cis-1-tert-butoxycarbonyl-3-triethylsilyloxy-4-(2-thienyl)azetidin-2-one, gave a triethylsilyl-protected, taxol-derived ester as primarily the (2'R,3'S)-isomer, together with a small amount of (2'S,3'R)-isomer. The mixture was deprotected with HF and pyridine in MeCN to give 91% 3'-desphenyl-3'-(2-thienyl)-N-desbenzoyl-(N-tert-butoxycarbonyl)-10-desacetoxytaxol (I). The other taxane derivs. were similarly prepared from protected azetidinones and baccatin (III) derivs. In an in vitro test against human colon carcinoma cells HCT-116, all I were said to have antiproliferative IC50 < 0.1 (no units), indicating cytotoxic activity.

IT **159406-32-3P 159406-33-4P 159406-34-5P**
159406-35-6P 159406-36-7P 159406-37-8P
159406-38-9P 159406-39-0P 159406-40-3P
159406-41-4P 159406-42-5P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; preparation of C-10 taxane derivs. as antileukemia and antitumor agents)

RN 159406-32-3 CAPLUS

JP 08505627	T2	19960618	JP 1994-516328		19940114
EP 1211250	A1	20020605	EP 2002-5075		19940114
EP 1211250	B1	20040616			
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PT 679082	T	20030228	PT 1994-909453		19940114
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AT 269315	E	20040715	AT 2002-5075		19940114
PT 1211250	T	20041029	PT 2002-5075		19940114
ES 2225671	T3	20050316	ES 2002-5075		19940114
CN 1495177	A	20040512	CN 2003-2003157907		19940115
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ES 2179070	T3	20030116	ES 1994-909840		19940301
IL 108836	A1	20051120	IL 1994-108836		19940303
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ZA 9401899	A	19941018	ZA 1994-1899		19940317
ZA 9401935	A	19941018	ZA 1994-1935		19940318
EP 1227093	A2	20020731	EP 2002-9840		19940321
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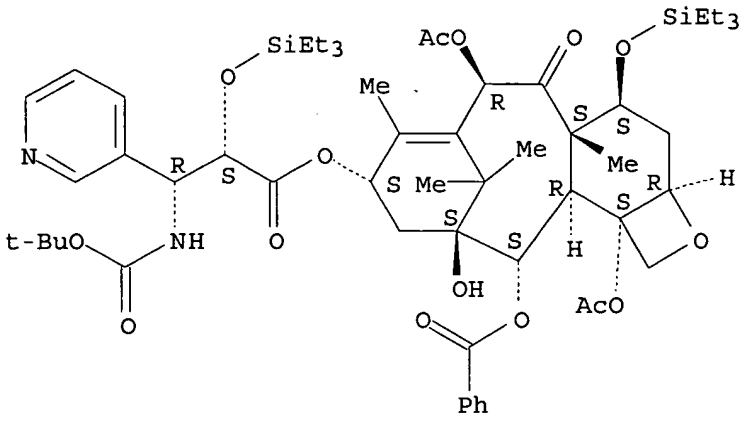
PRIORITY APPLN. INFO.:			US 1993-5229	A	19930115



IC ICM A61K031-335
ICS A61K031-44; C07D405-12; C07D305-14
INCL 514337000
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1, 63
IT 175840-97-8P 175840-98-9P 175841-00-6P **176017-80-4P**
176017-81-5P 176017-82-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and pharmaceutical compns. of taxanes having a pyridyl substituted side-chain)

L49 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:219064 CAPLUS
DOCUMENT NUMBER: 122:187818
TITLE: C-10 Taxane derivatives and pharmaceutical compositions containing them as antileukemia and antitumor agents
INVENTOR(S): **Holton, Robert A.**; Chai, Ki Byung
PATENT ASSIGNEE(S): Florida State University, USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9415599	A1	19940721	WO 1994-US479	19940114
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CA 2153805	AA	19940721	CA 1994-2153805	19940114
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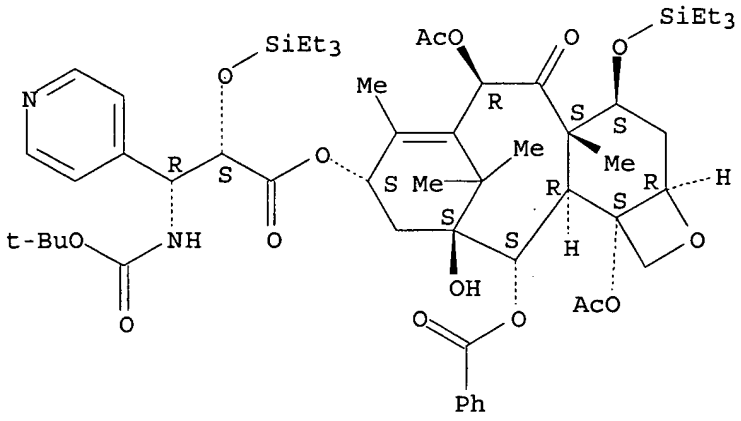
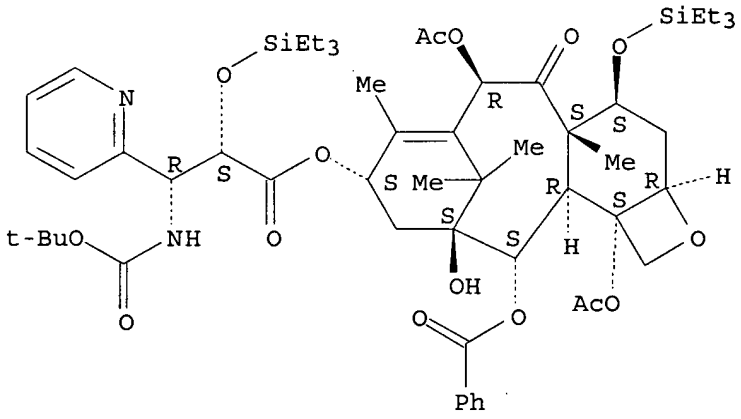
CA 2153903	AA	19940721	CA 1994-2153903	19940114
CA 2153903	C	20041102		
AU 9462295	A1	19940815	AU 1994-62295	19940114
AU 682852	B2	19971023		
EP 679082	A1	19951102	EP 1994-909453	19940114
EP 679082	B1	20021009		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				



RN 176017-81-5 CAPLUS
CN 2-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 176017-82-6 CAPLUS
CN 3-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

JP 1993-506299	A3	19920922
US 1992-967998	B1	19921026
US 1992-968003	A3	19921026
US 1993-34852	A	19930322
US 1993-95085	A	19930720
WO 1994-US2382	W	19940304
WO 1994-US3094	W	19940321
US 1994-263270	B1	19940621
US 1994-314532	A1	19940928
US 1994-351532	A3	19941207
US 1995-483309	A3	19950607
US 1995-516299	B1	19950817
US 1996-607108	A1	19960226
US 1997-941640	A1	19970930
US 2000-517791	A1	20000302
US 2000-566970	A1	20000509
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US 2002-289103	A1	20021106

OTHER SOURCE(S): MARPAT 124:317534

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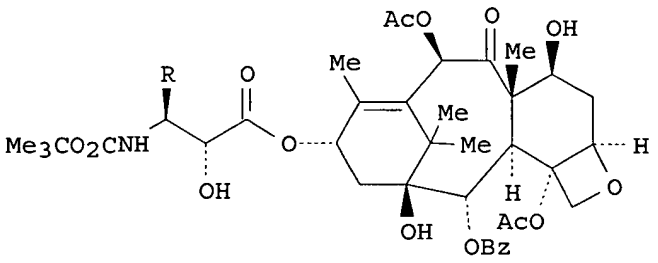

I

AB Taxane derivs. having a 3' pyridyl substituted C13 side chain, e.g. I (R = 2-, 3-, 4-pyridyl) were prepared as anticancer agents. Thus, 7-triethylsilylbaccatin III was treated with cis-1-(tert-butoxycarbonyl)-3-triethylsilyloxy-4-(4-pyridyl)azetidin-2-one followed by desilylation with HF to give I (R = 4-pyridyl). All I had an IC50 of less than 0.1, indicating they are cytotoxically active.

IT **176017-80-4P 176017-81-5P 176017-82-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and pharmaceutical compns. of taxanes having a pyridyl substituted side-chain)

RN 176017-80-4 CAPLUS

CN 4-Pyridinepropanoic acid, β-[[(1,1-dimethylethoxy)carbonyl]amino]-α-[(triethylsilyl)oxy]-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αS*,βR*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE					
CZ 287417	B6	20001115	CZ 1994-660		19920922
CZ 287609	B6	20010117	CZ 1994-661		19920922
EP 1193252	A2	20020403	EP 2002-688		19920922
EP 1193252	A3	20031105			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE					
SG 97130	A1	20030718	SG 1999-4181		19920922
CN 1075315	A	19930818	CN 1992-112286		19920923
CN 1048982	B	20000202			
US 5430160	A	19950704	US 1993-34247		19930322
CA 2158863	AA	19940929	CA 1994-2158863		19940321
WO 9421252	A1	19940929	WO 1994-US3094		19940321
W: AU, CA, CN, CZ, FI, HU, JP, KR, NO, NZ, PL, RU					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
AU 9465229	A1	19941011	AU 1994-65229		19940321
AU 684768	B2	19980108			
EP 690712	A1	19960110	EP 1994-912838		19940321
EP 690712	B1	20011128			
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JP 08508471	T2	19960910	JP 1994-521329		19940321
AT 209489	E	20011215	AT 1994-912838		19940321
ES 2164100	T3	20020216	ES 1994-912838		19940321
PT 690712	T	20020531	PT 1994-912838		19940321
TW 396159	B	20000701	TW 1994-83103422		19940418
US 5574156	A	19961112	US 1994-254561		19940606
TW 438772	B	20010607	TW 1994-83105964		19940630
US 5539103	A	19960723	US 1994-351532		19941207
US 5723634	A	19980303	US 1995-483309		19950607
US 6066747	A	20000523	US 1995-522307		19951030
US 5760219	A	19980602	US 1996-717136		19960920
US 6069260	A	20000530	US 1997-941640		19970930
AU 9856373	A1	19980430	AU 1998-56373		19980302
AU 702492	B2	19990225			
US 6479678	B1	20021112	US 2000-517791		20000302
US 2001014746	A1	20010816	US 2001-804821		20010313
US 6562962	B2	20030513			
US 2003027855	A1	20030206	US 2002-208418		20020730
US 6710191	B2	20040323			
US 2003120096	A1	20030626	US 2002-289103		20021106
US 6683196	B2	20040127			
JP 2004043439	A2	20040212	JP 2003-128200		20030506
US 2004073048	A1	20040415	US 2003-673897		20030929
US 7074945	B2	20060711			
PRIORITY APPLN. INFO.:			US 1991-763805	B2	19910923
			US 1992-862955	B2	19920403
			US 1992-863849	B2	19920406
			US 1992-949107	B2	19920922
			US 1993-34247	A2	19930322
			US 1989-359634	YY	19890531
			US 1989-415028	A1	19890929
			US 1992-862778	A2	19920403
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			US 1992-863840	A	19920406
			US 1992-900408	A	19920618
			CA 1992-2077394	A3	19920902
			CA 1992-2098478	A3	19920922
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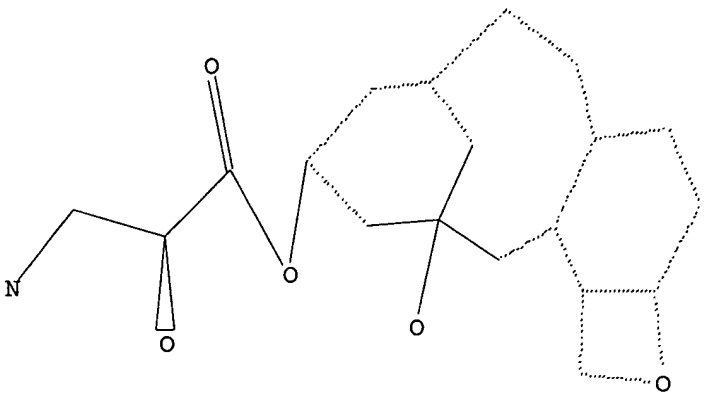

Structure attributes must be viewed using STN Express query preparation.

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L24           59 SEA FILE=CAPLUS ABB=ON  PLU=ON  L22
L44           51 SEA FILE=REGISTRY ABB=ON  PLU=ON  11R AND L5
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L46            3 SEA FILE=CAPLUS ABB=ON  PLU=ON  HOLTON R A/AU
L47           99 SEA FILE=CAPLUS ABB=ON  PLU=ON  HOLTON ROBER?/AU
L49            7 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L45 OR L24) AND (L46 OR L47)
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=> d ibib abs hitstr hitind L49 1-7

L49 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:169149 CAPLUS
DOCUMENT NUMBER: 124:317534
TITLE: Preparation and pharmaceutical compositions of taxanes having a pyridyl substituted side-chain
INVENTOR(S): **Holton, Robert A.**; Rengan, Kasthuri
PATENT ASSIGNEE(S): Florida State University, USA
SOURCE: U.S., 19 pp. Cont.-in-part of U.S. 5,430,160.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 28
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5489601	A	19960206	US 1993-95085	19930720
CA 2221190	AA	19920902	CA 1992-2221190	19920902
CA 2221190	C	20020212		
ZA 9206827	A	19930315	ZA 1992-6827	19920908
ZA 9206828	A	19930315	ZA 1992-6828	19920908
ZA 9206829	A	19930315	ZA 1992-6829	19920908
ZA 9207038	A	19930514	ZA 1992-7038	19920915
ZA 9207039	A	19931220	ZA 1992-7039	19920915
IL 103191	A1	20010724	IL 1992-103191	19920916
CA 2254273	AA	19920922	CA 1992-2254273	19920922
CA 2254273	C	20030325		
EP 884314	A2	19981216	EP 1998-114788	19920922
EP 884314	A3	20020502		
EP 884314	B1	20040121		

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AUTHOR SEARCH

FILE COVERS 1907 - 19 Sep 2006 VOL 145 ISS 13
FILE LAST UPDATED: 18 Sep 2006 (20060918/ED)

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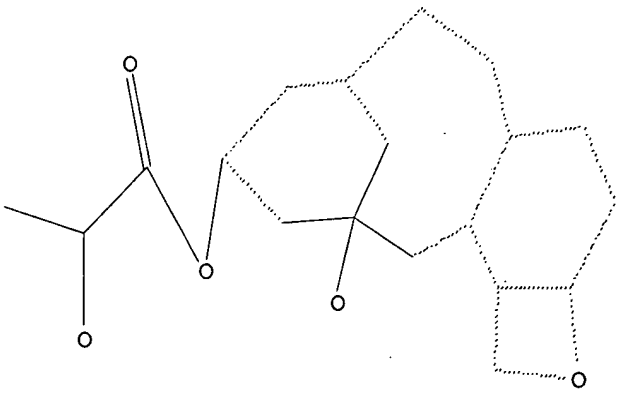
http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L49

L3 STR



Structure attributes must be viewed using STN Express query preparation.
L5 7665 SEA FILE=REGISTRY SSS FUL L3
L20 STR

4 (Parity=Even)

Stereo RSS Sets:

Type=Absolute (Default). 1 Nodes= 4

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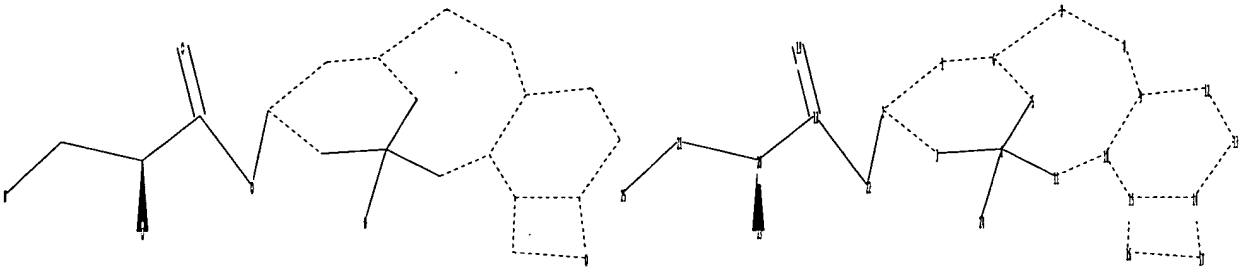
Uploading L20.str



chain nodes :
18 19 20 22 23 24 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
ring/chain nodes :
21
chain bonds :
2-22 4-24 18-20 18-19 18-22 20-21 20-23 21-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-11 5-6 6-7 7-8 8-9 9-10 9-12 10-11 10-15 12-13
13-14 14-15 14-17 15-16 16-17
exact/norm bonds :
1-2 1-6 2-3 2-22 3-4 4-5 4-11 4-24 5-6 6-7 7-8 8-9 9-10 9-12 10-11
10-15 12-13 13-14 14-15 14-17 15-16 16-17 18-19 18-22 20-23 21-25
exact bonds :
18-20 20-21

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

Stereo Bonds:

23-20 (Single Wedge).

Stereo Chiral Centers:

20 (Parity=Odd)

Stereo RSS Sets:

Type=Absolute (Default). 1 Nodes= 20

exact/norm bonds :
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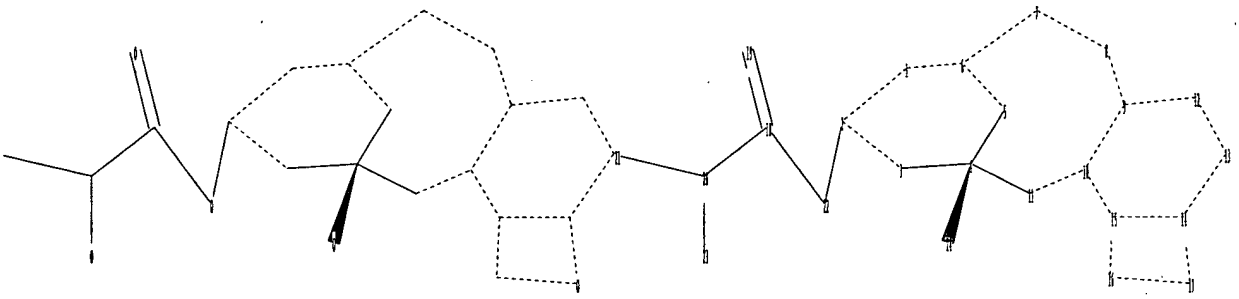
10-15 12-13 13-14 14-15 14-17 15-16 16-17 18-19 18-22 20-23
exact bonds :
18-20 20-21

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

Structure L14:

Uploading L14.str



chain nodes :
18 19 20 22 23 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
ring/chain nodes :
21
chain bonds :
2-22 4-24 18-20 18-19 18-22 20-21 20-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-11 5-6 6-7 7-8 8-9 9-10 9-12 10-11 10-15 12-13
13-14 14-15 14-17 15-16 16-17
exact/norm bonds :
1-2 1-6 2-3 2-22 3-4 4-5 4-11 4-24 5-6 6-7 7-8 8-9 9-10 9-12 10-11
10-15 12-13 13-14 14-15 14-17 15-16 16-17 18-19 18-22 20-23
exact bonds :
18-20 20-21

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

Stereo Bonds:

24-4 (Single Hash).

Stereo Chiral Centers:

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=> file registry
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DICTIONARY FILE UPDATES:  18 SEP 2006  HIGHEST RN 907539-37-1

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on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Structures searched:

Structure L3:

Uploading L3.str
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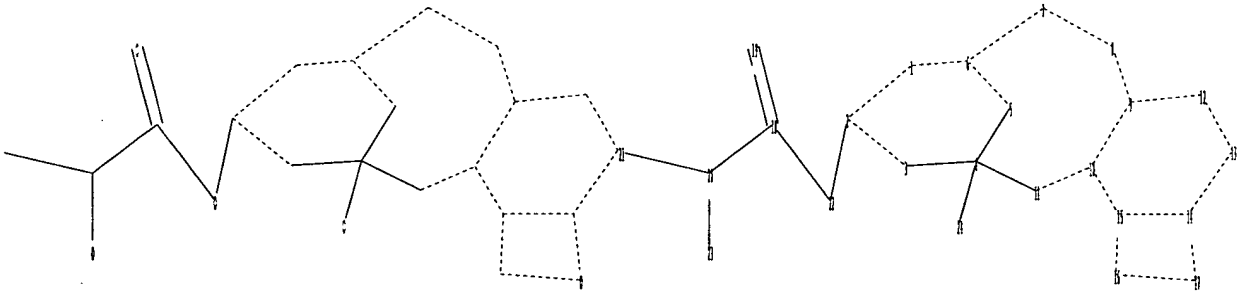

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chain nodes :
18  19  20  22  23  24
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17
ring/chain nodes :
21
chain bonds :
2-22  4-24  18-20  18-19  18-22  20-21  20-23
ring bonds :
1-2  1-6  2-3  3-4  4-5  4-11  5-6  6-7  7-8  8-9  9-10  9-12  10-11  10-15  12-13
13-14  14-15  14-17  15-16  16-17
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